ABSTRACT

Title of Dissertation: A Modified Zwanzig-Mori Formalism

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Recent advances in science have led to a better understanding of physical phenomena across a vast range of time and length scales. This has given the research community access to mathematical models for most scales in a given problem. A common strategy applied to Hamiltonian systems has been to select scales of interest and remove the others through the Zwanzig-Mori formalism. As long as the scales involved are strongly separated this approach works well. However, many problems in science and engineering involve processes in which there is no clear scale separation. It is still possible to use this procedure in some such cases but it has notably failed in many others (e.g. complex fluids). This failure has been blamed on the presence of poorly understood empirical closures and much current work is dedicated to eliminating the need for these or at least quantifying the errors they introduce.

I have constructed a model system that possesses many of the features present in relevant problems and have used it as a testbed for investigating a modification of the Zwanzig-Mori formalism. The modified formalism I propose is applicable beyond the standard class of Hamiltonian systems: it is designed to work with damped, noise-driven, Hamiltonian systems. This thesis describes the modest first steps in understanding the underlying functional analytic structure of the new formalism.

In particular, I have placed the model into a hierarchy of systems related to one another by a map between scales. The scale connection between the hierarchy elements is made evident by the construction of an intrinsic entropy-based fluid moment system—each element of the hierarchy is realized as a formal coarsening of this fluid moment system. What is more, I have formally constructed the "infinite particle" limit for the fluid moment system and found that it too has an associated entropy. The existence of these entropies implies an amenability of the new formalism to analysis—this is the most useful and novel aspect of the work.

A Modified Zwanzig-Mori Formalism

by

J.T. Halbert

Dissertation submitted to the Faculty of the Graduate School of the
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Preface

Give me a fruitful error any time, full of seeds, bursting with its own corrections. You can keep your sterile truths for yourself.

Vilfredo Pareto

The generic can be more intense than the concrete.

J.L. Borges

Be brave. Clench fists.

The Streets

DEDICATION

This is for Deanne and Shepherd.

ACKNOWLEDGEMENTS

I have been enamoured of hyperbole my entire life and wherever this thesis is circumspect I assure the reader I have there successfully suppressed my natural instinct toward exaggeration. Having said that, I must further assure the reader that however much I free myself from the constraints of scientific language in this section my effusiveness will be inadequate. This work would not have happened but for the help, encouragement, and patience of a great many people. In the following paragraphs I will express my gratitude as clearly as I can.

My advisor, Dr. David Levermore initially drew me to this problem with a few discussions about the importance of scaling in physical systems. My interest in the topic has not waned and it is due in large part to his willingness to indulge my taste for wide-ranging conversation. These talks coursed from the details of fluid dynamics to speculations on economics and were entertaining and invigorating.

Often they took a turn for the Socratic, and this mode is how most of the work on this thesis was accomplished. Dr. Levermore's willingness to let me make significant mistakes and correct them myself has made me a better researcher.

I must of course thank my committee for their generous donation of time and energy to my graduate career.

Dr. Stuart Antman gave detailed writing advice and pointed out important gaps in my knowledge. Dr. Dio Margetis' commentary on my initial draft of this work was incredibly valuable. The questions he raised about my work have improved it. Dr. Dmitry Dolgopyat's clear and precise writing, particularly on the topic of averaging, has served as a model for my own writing. I hope I am not flattering myself overmuch when I interpret his singularly brief commentary on my thesis as approval. Dr. Christopher Lobb is an inspiring lecturer and the person from whom I learned statistical mechanics. In my own teaching I have tried to emulate him. His general scientific questions about my work have helped me place it in its proper context.

The staff of the Mathematics department have been unfailingly helpful. In particular I would like to thank Alverda McCoy who took the trouble to forget that I was not a member of AMSC and helped me often.

I would not have made it this far except for the excellent undergraduate training I received at the University of Texas at Austin. In particular I would like to thank Dr. Maruthi Akella for introducing me to technical scientific work and Dr. Rafael de la Llave for his encouragement. Dr. de la Llave helped me when I needed it most.

I will resist the urge to quote Epicurus about friends. I have been lucky enough to have many of them. All of them are interesting, loyal, and good.

I was encouraged by and learned a great deal from many of my fellow graduate students at the University of Maryland. In particular Avanti Athreya, Hyejin Kim, Kostas Spiliopoulos, and Aliza Steurer were invaluable.

Chris Danforth and Aaron Lott were my office mates for too short a time. They taught me a great deal about leadership and how to achieve complex objectives as a team. My favorite times in graduate school where the conversations we had in our windowless dungeon.

This time in graduate school has been made immeasurably easier by the McCormick family. Neil and Ruth Anne, and their daughters Emily and Elizabeth adopted us shortly after our arrival. They invited us into their home and through the years have become our second family.

The penultimate expression must go to my oldest and best friend. Jason James has been consistently inspiring through many adventures—both those that deserve the name and more common endeavors. I have always been proud to be called his friend. I could not have done this without his encouragement.

Finally, and most importantly, I would like to thank my wife Deanne and my son Shepherd. Deanne is the strongest, wisest, and kindest

person I know. She has a natural instinct for justice and the good, and I can always rely on her help. Whenever I am contented least with what I enjoy most she calmly leads me through. I could not live without her. What can I say about our perfect little Shepherd? I think it will always feel like he came to us "not long ago". He is a joy and the days fly by.

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Introduction

Recent advances in science have led to a better understanding of physical phenomena across a vast range of time and length scales. This has given the research community access to mathematical models for most scales in a given problem. However, many problems in science and engineering involve processes in which there is no clear separation of these scales (e.g. modeling a fusion reactor or the climate), and while good models may exist for the component levels of description, there is no obvious way to simulate or understand the whole from knowledge of the parts in this case. New mathematics is required to tell researchers how to integrate different models over a range of scales. [15]

One approach to synthesis between scales is the class of "dimensional reduction methods". In the 60s and 70s, Zwanzig [35–37] and Mori [28] developed formal projection techniques that could be used to derive effective "coarse-grained" equations for the statistical properties of many out-of-equilibrium Hamiltonian systems. More recently, Chorin et al. [6,8–13] have applied various closures to the Zwanzig-Mori formalism to develop dimensional reduction techniques. The goal is always to take high-dimensional, detailed models and reduce their complexity by integrating out (in a systematic way) the "unimportant" degrees of freedom or modes.

E and Engquist [16] point out that standard reduction methods must often be empirically closed. That is, there will be parameters in the reduced model that depend in an unknown way on the micro-scale model and must be handled separately by physical experiment or an appeal to a different model. E and Engquist make use of the Zwanzig-Mori formalism to develop new techniques that can consolidate micro-scale models directly into the macro-scale models instead of having to rely on empirical modeling.

This is the frontier in multi-scale modeling: the so-called "first principles" approach. Models are built from the smallest scale up and the goal is to produce the macro-scale parameters directly from the micro-scale instead of having to rely on empirical closures. The detailed understanding of such an approach is just beginning and it is this setting in which I have made my modest contribution. As a first step I have developed an inherently multi-scale model that is convenient analytically. It is a damped, noise driven, Hamiltonian system given as a collection of stochastic differential equations. I have used this model as a testbed for investigating a modification of the Zwanzig-Mori formalism.

The modification I propose is based on a "hierarchy of models" approach. That is, one considers a given model for a physical system and a map from that model to coarsened versions of it. Iteration of this map, coupled with an appropriate way of moving from a coarse to a fine picture, is akin to the renormalization group[1] notion from statistical mechanics. In the case I describe the entire hierarchy can be realized through a novel system of integro-differential equations that

[1]For background on the view from the physics community of the renormalization group see [20] for an excellent short discussion, or [22] for a more pedagogical presentation.

have a fluid system as a formal limit. Formally this limit is the fixed point of the hierarchy map.

This investigation is a first step in understanding the functional analytic structure of the maps between scales in a given problem. Additionally, it serves as an extension of the Zwanzig-Mori formalism into a non-Hamiltonian setting.

1.1 Plan of Thesis

Some of the work in this thesis is formal or incomplete. This is due to the nature of the problem and the constraints of time and ability. I will make a good faith attempt to point out where I am being formal and where holes exist in arguments. The thesis is organized as follows.

Chapter 2 is a presentation of our model system. The model has been constructed to capture as many features of multi-scale systems as possible while still being analytically tractable. It is somewhat physically relevant—though this is not its reason for being—in the sense that it mimics the structure of existing models of polymers. It consists of a system of stochastic differential equations with an associated Kolmogorov equation describing the evolution of the phase space density. The majority of the chapter will be devoted to the properties (both formal and rigorous) of this associated Kolmogorov equation. The contents are for the most part highly technical.

Chapter 3 contains the heart of the work (but not the soul). I will briefly review the Zwanzig-Mori formalism and the recent uses and clarifications of it and then introduce my proposed modification. The chapter will close with an application to a toy version of our model. This toy model examination will display the need for a hydrodynamic limit that is the topic for the last two chapters.

Chapter 4 contains the soul of the work. We will discuss the central novelty: the construction of a system of partial integro-differential equations that describe the evolution of certain marginals of our evolving phase space density.

Chapter 5 is the most formal and incomplete. It contains a discussion of the hydrodynamic limit for our model. The discussion is essentially a list of open questions with a few notes on possible answers.

The thesis closes with an appendix containing supplemental material. This includes some necessary functional analysis and calculus as well as some details that would not have been profitable to read in the middle of the text.

Chapter 2

A Model Interacting Particle System

This chapter lays out in detail the model I have investigated. The model has been crafted to include as many interesting features of relevant physical systems as possible while still being analytically tractable. Our final system will be a collection of stochastic differential equations modeling N particles on a string interacting only with nearest neighbors. This system could also serve as a model for a polymer where each "particle" in our description would be some representation of the repeated structural units and the interaction potential would stand in for the covalent chemical bonds. The presence of the noise and damping would then be present to aid in simulation as in [25]. It is important to note, however, that this system has been developed as a testbed for a formalism, *not* to model any specific physical phenomena.

Associated with the system of stochastic differential equations will be a forward Kolmogorov equation governing the time evolution of the probability density for the system. I will discuss the properties of this equation in some detail in this chapter. In particular, the appropriate Sobolev spaces will be defined and the existence of an invariant measure will be discussed. Additionally, we will see that the system admits an entropy that is dissipated by the dynamics. This discussion sets the stage for the new formalism proposed in Chapter 3.

2.1 Our System

The model I consider is a necklace formation of N particles. Figure 2.1 is meant to convey the idea. The particles are constrained to move on a circle and interact only with their nearest neighbors.

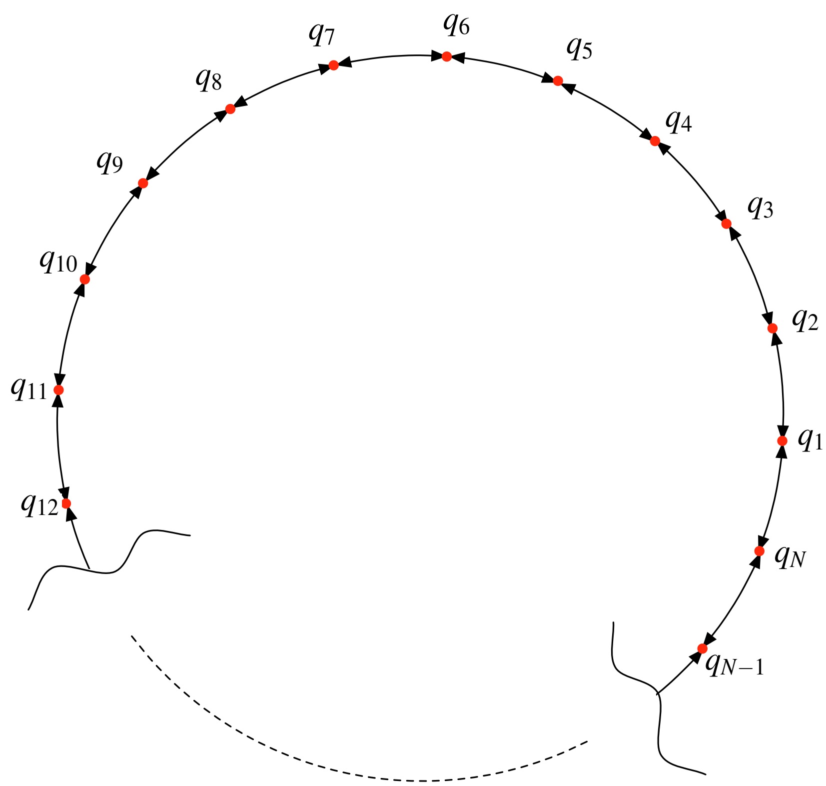

Figure 2.1: A necklace of interacting particles

The model is based on dissipative particle dynamics. In particular, the setting comes from the work of Español [17], and Hoogerbrugge and Koelman [25] via an example illustrated in recent work by Eyink and Levermore [19]. The general idea is that noise and damping is added "between particles" so as to conserve momentum. This approach was originally developed in order to give a less computationally intensive route to the simulation of fluid equations. It entails discarding usual notions of "particles" since the form of the noise and damping means that we are treating our system elements as "parcels": groups of particles whose internal behavior is unknown. This notion will be clarified below and in Section 3.5.2; for now, we will continue with the convenient particle idea.

2.1.1 Particle Dynamics

Consider N point particles moving on the circle $\mathbb{T} = \mathbb{R}/\mathbb{Z}$. Let $\boldsymbol{q} = (q_1, q_2, \ldots, q_N)$ be the vector of particle positions and $\boldsymbol{p} = (p_1, p_2, \ldots, p_N)$ be the vector of associated momenta. The details of the phase space for this system will be discussed in Section 2.1.2.

We start by assuming the particles have an associated Hamiltonian

$$H(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{2}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p} + \varPhi(\boldsymbol{q})\,, \tag{2.1.1}$$

where $\boldsymbol{M}$ is a diagonal mass matrix with $\boldsymbol{M}_{ii} = m_i$ interpreted as the mass of the i^{th} particle, and $\varPhi$ is a nearest-neighbor interaction potential

$$\varPhi(\boldsymbol{q}) = \sum_{i=1}^{N} \phi_{i-1/2}(q_i - q_{i-1})\,. \tag{2.1.2}$$

The peculiar subscript is meant to indicate that the potential $\phi_{i-1/2}$ couples particle i and particle $i-1$, where $q_0 = q_{N-1}$. The form of the individual particle interactions $\phi_{i-1/2}$ will be left open for now. Later it will prove convenient to posit power-law interactions. Suffice it now to assume $\phi_{i-1/2}$ is smooth and satisfies

$$\lim_{s\to 0} \phi_{i-1/2}(s) = \infty\,. \tag{2.1.3}$$

This is enough to ensure the particles do not pass through one another in the Hamiltonian setting. It will be necessary in Section 3.5.2 to relax this assumption.

The assumption of nearest-neighbor interactions requires some justification. It is connected to the "parcel" notion mentioned above. In any realistic particle system any individual particle will interact with all the others. But, here we are working with the idea that the interacting components are really parcels. The unmodeled particles in these parcels may interact with all others but the force due to an element of another parcel will necessarily be weak.[1] This means that the neighboring parcels' interaction will be dominated by the interactions of their "edge" members. Add to this the idea of repeated clumping of parcels into larger collections (renormalization) and the effect becomes even more pronounced. Hence, the assumption of nearest-neighbor interaction is a natural modeling compromise.

The effect of unmodeled particles is taken into account by adding noise and damping. The size of the noise must be controlled so that the added impetus does not force the particles over the potential energy barrier. This issue is deep and has not been fully resolved. After introducing the equations I will discuss it in Remark 2.1.1.

Our particles are required to obey the system of stochastic differential equations

$$d\boldsymbol{q} = \nabla_{\boldsymbol{p}} H dt \,, \tag{2.1.4}$$

$$d\boldsymbol{p} = -\nabla_{\boldsymbol{q}} H dt - \boldsymbol{\Xi} \nabla_{\boldsymbol{p}} H dt + \sqrt{2\theta}\boldsymbol{\Omega}^T \boldsymbol{\Lambda} d\boldsymbol{W} \,, \tag{2.1.5}$$

[1] This is true if we make the standard assumption that the potential decays.

where $\boldsymbol{\Xi} = \boldsymbol{\Omega}^T \boldsymbol{\Lambda}^2 \boldsymbol{\Omega}$,

$$\boldsymbol{\Omega} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & -1 \\ -1 & 1 & 0 & \ddots & 0 & 0 \\ 0 & -1 & 1 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \ddots & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix}, \tag{2.1.6}$$

and $\boldsymbol{\Lambda}$ is an $N \times N$ diagonal matrix with $\boldsymbol{\Lambda}_{ii} = \lambda_{i-1/2}(q_i - q_{i-1})$ some as-yet-unspecified function $\lambda_{i-1/2}$ representing the strength of the noise between particles. The noise term $d\boldsymbol{W}$ is a vector of N independent Brownian motion increments[2] and θ has a natural interpretation as the temperature for our system. This choice of noise and damping has the useful property of giving the system an exponential equilibrium distribution (see Section 2.2).

Remark 2.1.1. Physically it is apparent that the strength of the noise between particles must be moderated by the strength of the potential energy that keeps them separate. After all, should the noise grow as the particles come together it is possible that it would push them across the potential energy barrier. We must place restrictions on the noise strength so that this does not happen. A full answer is beyond the scope of this thesis but I will provide heuristics for the scaling relation between the potential energy and the noise strength.

Consider the following illustrative scenario. Place a particle in the power law potential well

$$\phi(x) = \frac{1}{(1-x)^\gamma} + \frac{1}{x^\gamma}, \tag{2.1.7}$$

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[2] See Øksendal [29] for an elementary discussion of Brownian motion, or Karatzas and Shreve [26] for a more detailed look.

and add noise of variable strength so that the particle position x is governed by the one-dimensional stochastic differential equation

$$dx = -\phi'(x)dt + \lambda(x)dW\,. \tag{2.1.8}$$

Notice that if $\lambda \equiv 0$ then the particle oscillates in the interval $(0,1)$, never reaching 0 or 1. What constraints must be placed on λ so that the probability of the particle reaching 0 or 1 remains zero?

It is possible, in this simple setting, to answer this question precisely using standard tools from stochastic processes. We apply what is known as the Feller test. Consult chapter 6 of [34] for the details. In brief we consider the generator

$$L = -\phi'(x)\frac{d}{dx} + \frac{1}{2}\lambda^2(x)\frac{d^2}{dx^2} \tag{2.1.9}$$

for this simple diffusion on $(0,1)$. We define stopping times $\tau_c = \{\inf t : x(t) = c\}$, $\tau_0 = \lim_{c\searrow 0}\tau_c$, and $\tau_1 = \lim_{c\nearrow 1}\tau_c$. The probability of the particle reaching 1 (say) is precisely $P\left[\tau_1 < \infty\right]$. The Feller test is related to the solution u of

$$Lu = 0\,, \tag{2.1.10}$$

which is (by a straightforward calculation)

$$u(x) = \int_{1/2}^{x} \exp\left(-2\int_{1/2}^{y} \frac{-\phi'(z)}{\lambda^2(z)}\,dz\right)\,dy\,. \tag{2.1.11}$$

Now, Lemma 6.4 of [34] gives us the desired test:

$$\text{if} \quad \lim_{x\to 1}\int_{1/2}^{x} \exp\left(-2\int_{1/2}^{y} \frac{-\phi'(z)}{\lambda^2(z)}\,dz\right)\,dy = \infty \quad \text{then} \quad P\left[\tau_1 < \infty\right] = 0\,. \tag{2.1.12}$$

That is, the process will fail to reach 1 in finite time if a particular integral becomes unbounded. Now we can employ order estimates to obtain a relation between the allowed growth in λ given that $\phi = \mathcal{O}\left(\frac{1}{(1-z)^\gamma}\right)$ as $z \to 1$.

Suppose $\lambda^2 = \mathcal{O}((1-z)^\alpha)$ as $z \to 1$. This implies

$$\int_{1/2}^{y} \frac{2\phi'}{\lambda^2}\, dz = \int_{1/2}^{y} \mathcal{O}\!\left(\frac{1}{(1-z)^{\gamma+1+\alpha}}\right) dz = \mathcal{O}\!\left(\frac{1}{(1-y)^{\alpha+\gamma}}\right) . \tag{2.1.13}$$

Now

$$\lim_{x\to 1} \int_{1/2}^{x} \exp\left(\frac{1}{(1-y)^{\alpha+\gamma}}\right) dy = \infty \qquad \text{if } \alpha+\gamma > 0\,, \tag{2.1.14}$$

and so we know the following. If the potential energy ϕ grows as $1/(1-x)^\gamma$ when $x \to 1$ we must require that the noise strength λ grow slower than $1/(1-x)^{\gamma/2}$.

So, in an extremely simple case we know that it is possible to add noise while preserving the particle order. For the remainder of this thesis we will assume the functions $\lambda_{i-1/2}$ scale appropriately. These functions arise in practice through the matrix $\boldsymbol{\Xi}$. Section A.4 is dedicated to it. Suffice it to say here that $\boldsymbol{\Xi}$ is positive semi-definite with

$$\mathrm{Null}\,(\boldsymbol{\Xi}) = \left\{ v \in \mathbb{R}^N \mid \boldsymbol{\Xi} v = 0 \right\} = \mathrm{span}\,\{\mathbf{1}\}\ ,$$

where $\mathbf{1} = (1, 1, \ldots, 1)$.

2.1.2 Phase Space

The configuration space $\mathcal{Q}$ for our N-particle system is an N-submanifold of $\mathbb{T}^N$. We put coordinates on it by choosing one particle as the marker and registering the position of the other particles by their separation from this tracer. It is made precise in the following definitions.

Definition 2.1.1. *Let* $\{e_j\} \subset \mathbb{R}^{N-1}$ *be the standard unit vectors and define* $\triangle^\circ_{N-1}$ *as the interior of the convex hull of the collection* $\{e_j\}_{j=1}^{N-1} \cup \{0\}$*. Equivalently*

$$\triangle^\circ_{N-1} = \left\{ \{s_2, \ldots, s_N\} \in \mathbb{R}^{N-1} \,\middle|\, s_i > 0, \sum_{i=2}^{N} s_i < 1 \right\}.$$

Note that $\overline{\triangle^\circ_{N-1}}$ *is the regular* $(N-1)$*-simplex.*

Definition 2.1.2. *Define* $\Psi_1 : \mathbb{S}^1 \times \triangle^\circ_{N-1} \to \mathbb{T}^N$ *as*

$$\Psi_1 (q_1, s_2, \ldots, s_N) = (q_1, q_1 + s_2, q_1 + s_2 + s_3, \ldots, q_1 + s_2 + \cdots + s_N) \mod 1 \,. \tag{2.1.15}$$

Lemma 2.1.1. Ψ_1 *is a diffeomorphism onto its image.*

Proof. Ψ_1 is a linear map with determinant 1. □

With Ψ_1 we can define (and simultaneously put coordinates on) the configuration space $\mathcal{Q}$ by making

Definition 2.1.3. $\mathcal{Q} = \mathrm{Range}\,(\Psi_1)$. *Note that this implies we can integrate over* $\mathcal{Q}$ *as follows.*

$$\int_{\mathcal{Q}} f(\boldsymbol{q})\, d\boldsymbol{q} = \int_{\triangle^\circ_{N-1}} \int_0^1 f\left(\Psi_1(q_1, s_2, \ldots, s_N)\right)\, dq_1 ds_2 \cdots ds_N \,, \tag{2.1.16}$$

with

$$\int_{\triangle^\circ_{N-1}} = \int_0^1 \int_0^{1-s_N} \int_0^{1-(s_{N-1}+s_N)} \cdots \int_0^{1-\sum_{k=j+1}^N s_k} \cdots \int_0^{1-\sum_{k=3}^N s_k} \,. \tag{2.1.17}$$

Now, the phase space for our particle motion is $\Gamma = \mathbb{R}^N \times \mathcal{Q}$.

2.1.3 Conserved Quantities

A straightforward calculation can verify that $d\sum_{i=1}^N p_i = 0$.

$$d\sum_{i=1}^N p_i = d\boldsymbol{p} \cdot \mathbf{1} = -\nabla_{\boldsymbol{q}} H \cdot \mathbf{1} - \boldsymbol{\Xi} \nabla_{\boldsymbol{p}} H \cdot \mathbf{1} + \sqrt{2\theta}\boldsymbol{\Omega}^T \boldsymbol{\Lambda} d\boldsymbol{W} \cdot \mathbf{1} \,, \tag{2.1.18}$$

but as noted in equation (A.4.1) $\mathbf{1}$ generates the null space of $\boldsymbol{\Omega}$ and so the last two terms are clearly 0. The first term is zero because the total force in the necklace is 0, that is, the form of Φ makes $\nabla_{\boldsymbol{q}}\Phi \cdot \mathbf{1}$ a telescoping sum of periodic elements. Hence, the total momentum is conserved.

It is important to remark that the total energy is *not* conserved: using the standard Itô calculus we have

$$H = \Phi(\boldsymbol{q}) + \frac{1}{2}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p}\,, \tag{2.1.19}$$

$$dH = \nabla_{\boldsymbol{q}}\Phi \cdot d\boldsymbol{q} + \boldsymbol{M}^{-1}\boldsymbol{p} \cdot d\boldsymbol{p} + \frac{1}{2}d\boldsymbol{p} \cdot \boldsymbol{M}^{-1}d\boldsymbol{p} \tag{2.1.20}$$

$$\begin{aligned} &= \cancel{\nabla_{\boldsymbol{q}}\Phi \cdot \boldsymbol{M}^{-1}\boldsymbol{p}\,dt} \\ &\quad + \boldsymbol{M}^{-1}\boldsymbol{p} \cdot \left(\cancel{-\nabla_{\boldsymbol{q}}\Phi\,dt} - \boldsymbol{\Xi}\boldsymbol{M}^{-1}\boldsymbol{p}\,dt + \sqrt{2\theta}\boldsymbol{\Omega}^T\boldsymbol{\Lambda}d\boldsymbol{W}\right) \\ &\qquad + \frac{1}{2}2\theta d\boldsymbol{W} \cdot \boldsymbol{M}^{-1}\boldsymbol{\Xi}d\boldsymbol{W} \end{aligned} \tag{2.1.21}$$

$$= \left[\theta \mathrm{tr}\left(\boldsymbol{M}^{-1}\boldsymbol{\Xi}\right) - \boldsymbol{M}^{-1}\boldsymbol{p} \cdot \boldsymbol{\Xi}\boldsymbol{M}^{-1}\boldsymbol{p}\right]\,dt + \sqrt{2\theta}\boldsymbol{M}^{-1}\boldsymbol{p} \cdot \boldsymbol{\Omega}^T\boldsymbol{\Lambda}d\boldsymbol{W}\,. \tag{2.1.22}$$

That is, the energy fluctuates in a known way. The investigation of the energy for our system is intriguing but is beyond the scope of this thesis.

2.2 Evolution of Probability Density

Let $F = F(\boldsymbol{p}, \boldsymbol{q}, t)$ be the probability density for our system. That is,

$$\int_B F\,d\boldsymbol{p}\,d\boldsymbol{q} = P\left[(\boldsymbol{p}(t), \boldsymbol{q}(t)) \in B\right]\,, \tag{2.2.1}$$

where $(\boldsymbol{p}(t), \boldsymbol{q}(t))$ is a solution to the collection (2.1.4), (2.1.5). It is well-known [21, 29] that the evolution of F is governed by a forward Kolmogorov equation that takes the form of the Fokker-Planck equation

$$\partial_t F + \boldsymbol{M}^{-1}\boldsymbol{p} \cdot \nabla_{\boldsymbol{q}}F - \nabla_{\boldsymbol{q}}\Phi \cdot \nabla_{\boldsymbol{p}}F = \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\left(\theta\nabla_{\boldsymbol{p}}F + \boldsymbol{M}^{-1}\boldsymbol{p}F\right)\right]\,. \tag{2.2.2}$$

The form of the right-hand side will prove convenient and is a partial justification for the form of the damping and noise in our model. For some of the following discussion it will be convenient to have a short form of this equation. We will write

$$\partial_t F = \mathcal{L}F = \mathcal{L}_A F + \mathcal{L}_S F\,, \tag{2.2.3}$$

where

$$\mathcal{L}_A F = \nabla_{\boldsymbol{q}} \varPhi \cdot \nabla_{\boldsymbol{p}} F - \boldsymbol{M}^{-1}\boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} F, \tag{2.2.4}$$

$$\mathcal{L}_S F = \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\varXi}\left(\theta \nabla_{\boldsymbol{p}} F + \boldsymbol{M}^{-1}\boldsymbol{p}F\right)\right]\,. \tag{2.2.5}$$

$\mathcal{L}_A$ will be referred to as the anti-symmetric part of $\mathcal{L}$ and $\mathcal{L}_S$ as the symmetric part. The reason for this will be shown below.

2.2.1 Formal Properties

The discussion of this section begins with the null space of $\mathcal{L}$. This is done to establish the existence of an invariant density which will be used in the discussion to follow.

Lemma 2.2.1. *The null space of* $\mathcal{L}$, $\mathrm{Null}(\mathcal{L})$*, contains the collection*

$$\left\{ f(\boldsymbol{p}\cdot\boldsymbol{1}) \exp\left(-\frac{1}{\theta}\left(\frac{1}{2}\boldsymbol{p}\cdot\boldsymbol{M}^{-1}\boldsymbol{p} + \varPhi\left(\boldsymbol{q}\right)\right)\right) \text{ where } f \text{ is nice.}\right\} \tag{2.2.6}$$

The qualification "nice" will make more sense below once we define $\mathrm{Dom}\left(\mathcal{L}\right)$ *in that we must require* $\mathrm{Null}(\mathcal{L}) \subset \mathrm{Dom}(\mathcal{L})$*.*

Proof. First consider the action of the symmetric part of $\mathcal{L}$:

$$\begin{aligned}\mathcal{L}_S\left[\exp\left(\frac{-1}{2\theta}\boldsymbol{p}\cdot\boldsymbol{M}^{-1}\boldsymbol{p}\right)\right] = \nabla_{\boldsymbol{p}} \cdot \Bigg[\boldsymbol{\varXi}\Bigg(\theta\left[-\frac{1}{\theta}\boldsymbol{M}^{-1}\boldsymbol{p}\exp\left(-\frac{1}{2\theta}\boldsymbol{p}\cdot\boldsymbol{M}^{-1}\boldsymbol{p}\right)\right] \\ + \boldsymbol{M}^{-1}\boldsymbol{p}\exp\left(-\frac{1}{2\theta}\boldsymbol{p}\cdot\boldsymbol{M}^{-1}\boldsymbol{p}\right)\Bigg)\Bigg] = 0\,. \end{aligned} \tag{2.2.7}$$

That does not exhaust the possibilities. Suppose

$$F = f(\boldsymbol{p}, \boldsymbol{q}) \exp\left(\frac{-1}{2\theta}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p}\right) . \tag{2.2.8}$$

We then have

$$\mathcal{L}_S F = \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\left(\theta \nabla_{\boldsymbol{p}} F + \boldsymbol{M}^{-1}\boldsymbol{p}F\right)\right] = \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\left(\nabla_{\boldsymbol{p}} f\right) \theta \exp\left(\frac{-1}{2\theta}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p}\right)\right] , \tag{2.2.9}$$

which means F is in the null space of $\mathcal{L}_S$ if $\boldsymbol{\Xi}\nabla_{\boldsymbol{p}} f = 0$, that is, in view of equation (A.4.1), if $\nabla_{\boldsymbol{p}} f = g(\boldsymbol{p}, \boldsymbol{q})\mathbf{1}$ for some scalar function g. But, this then implies that the $\boldsymbol{p}$ dependence of f is of a particular form:

$$f = f(\boldsymbol{p} \cdot \mathbf{1}, \boldsymbol{q}) . \tag{2.2.10}$$

Hence, we have F in the null space of $\mathcal{L}_S$ if it has form

$$F = f(\boldsymbol{p} \cdot \mathbf{1}, \boldsymbol{q}) \exp\left(\frac{-1}{2\theta}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p}\right) \tag{2.2.11}$$

$$= f(\boldsymbol{p} \cdot \mathbf{1}, \boldsymbol{q}) \exp\left(-\frac{1}{\theta}\left(\frac{1}{2}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p} + \Phi\left(\boldsymbol{q}\right)\right)\right) \text{ without loss of generality.} \tag{2.2.12}$$

Now, for F to be in the null space of $\mathcal{L}_A$ we must require that F Poisson-commute with the Hamiltonian for our system $H = \frac{1}{2}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p} + \Phi\left(\boldsymbol{q}\right)$, that is, we must require

$$\nabla_{\boldsymbol{q}}\Phi \cdot \nabla_{\boldsymbol{p}} F - \boldsymbol{M}^{-1}\boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} F = \nabla_{\boldsymbol{q}} H \cdot \nabla_{\boldsymbol{p}} F - \nabla_{\boldsymbol{p}} H \cdot \nabla_{\boldsymbol{q}} F = 0 . \tag{2.2.13}$$

But $F = f \exp\left(-\frac{1}{\theta}H\right)$ and so we require

$$\nabla_{\boldsymbol{q}} H \cdot \nabla_{\boldsymbol{p}} F - \nabla_{\boldsymbol{p}} H \cdot \nabla_{\boldsymbol{q}} F = \left[\nabla_{\boldsymbol{q}} H \cdot \nabla_{\boldsymbol{p}} f - \nabla_{\boldsymbol{p}} H \cdot \nabla_{\boldsymbol{q}} f\right] \exp\left(-\frac{1}{\theta}H\right) = 0 , \tag{2.2.14}$$

that is,

$$\nabla_{\boldsymbol{q}} H \cdot \nabla_{\boldsymbol{p}} f - \nabla_{\boldsymbol{p}} H \cdot \nabla_{\boldsymbol{q}} f = \nabla_{\boldsymbol{q}}\Phi \cdot \mathbf{1}g - \left(\boldsymbol{M}^{-1}\boldsymbol{p}\right) \cdot \nabla_{\boldsymbol{q}} f = 0 . \tag{2.2.15}$$

Recall from the discussion of conserved quantities in Section 2.1.3 that $\nabla_{\boldsymbol{q}} \Phi \cdot \mathbf{1} = 0$. Because $\boldsymbol{p}$ and $\boldsymbol{q}$ are independent, the fact that $\left(\boldsymbol{M}^{-1}\boldsymbol{p}\right) \cdot \nabla_{\boldsymbol{q}} f = 0$ implies $\nabla_{\boldsymbol{q}} f = 0$. This establishes the claim. $\square$

Lemma 2.2.1 allows us to establish an invariant density up to total momentum (something we know is conserved, see Section 2.1.3). We define this global equilibrium as

$$\mathcal{G}_o(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{\sqrt{\det\left(2\pi\theta \boldsymbol{M}\right)} Z_o} \exp\left(-\frac{1}{\theta}\left(\frac{1}{2}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p} + \Phi\left(\boldsymbol{q}\right)\right)\right), \tag{2.2.16}$$

where

$$Z_o = \int\limits_{\mathcal{Q}} \exp\left(-\frac{1}{\theta}\Phi(\boldsymbol{q})\right) \, d\boldsymbol{q}\,. \tag{2.2.17}$$

With this equilibrium in hand we can define the space on which the probability density is evolving. First note that the right-hand side of equation (2.2.2) can be written in the so-called comparison form as

$$\mathcal{L}_S F = \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\left(\theta \nabla_{\boldsymbol{p}} F + \boldsymbol{M}^{-1}\boldsymbol{p} F\right)\right] = \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\theta \mathcal{G}_o \nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_0}\right)\right]. \tag{2.2.18}$$

Note that $\mathcal{L}_S$ is formally symmetric in $\mathbb{H} = L^2\left(1/\mathcal{G}_o\right)$:

$$\begin{aligned}
(\mathcal{L}_S f, g)_{\mathbb{H}} &= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left(\mathcal{L}_S f\right) \frac{g}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \\
&= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{f}{\mathcal{G}_0}\right)\right] \frac{g}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \\
&= -\int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left[\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{f}{\mathcal{G}_o}\right)\right] \cdot \nabla_{\boldsymbol{p}}\left(\frac{g}{\mathcal{G}_o}\right) \, d\boldsymbol{p} \, d\boldsymbol{q} \\
&= -\int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left[\nabla_{\boldsymbol{p}}\left(\frac{f}{\mathcal{G}_o}\right)\right] \cdot \left[\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{g}{\mathcal{G}_o}\right)\right] \, d\boldsymbol{p} \, d\boldsymbol{q} \qquad (\boldsymbol{\Xi} \text{ is symmetric}) \\
&= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{g}{\mathcal{G}_0}\right)\right] \frac{f}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} = (f, \mathcal{L}_S g)_{\mathbb{H}}\,.
\end{aligned} \tag{2.2.19}$$

It is also the case that $\mathcal{L}_A$ is formally anti-symmetric in $\mathbb{H}$:

$$\begin{aligned}
(\mathcal{L}_A f, g)_{\mathbb{H}} &= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} (\mathcal{L}_A f) \, \frac{g}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \\
&= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left[\nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} f - \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} f \right] \frac{g}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \\
&= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left[\nabla_{\boldsymbol{p}} \cdot (f \nabla_{\boldsymbol{q}} \Phi) - \nabla_{\boldsymbol{q}} \cdot \left(f M^{-1} \boldsymbol{p} \right) \right] \frac{g}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \\
&= - \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} f \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} \left(\frac{g}{\mathcal{G}_o} \right) - f \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} \left(\frac{g}{\mathcal{G}_o} \right) \, d\boldsymbol{p} \, d\boldsymbol{q} \, , \qquad (2.2.20)
\end{aligned}$$

and

$$\nabla_{\boldsymbol{p}} \left(\frac{g}{\mathcal{G}_o} \right) = \frac{\nabla_{\boldsymbol{p}} g}{\mathcal{G}_o} - \frac{1}{\mathcal{G}_o^2} \mathcal{G}_o \left(- \frac{\boldsymbol{M}^{-1} \boldsymbol{p}}{\theta} \right) = \frac{1}{\mathcal{G}_o} \left(\nabla_{\boldsymbol{p}} g + \frac{1}{\theta} \boldsymbol{M}^{-1} \boldsymbol{p} \right) , \qquad (2.2.21)$$

$$\nabla_{\boldsymbol{q}} \left(\frac{g}{\mathcal{G}_o} \right) = \frac{1}{\mathcal{G}_o} \left(\nabla_{\boldsymbol{q}} g + \frac{1}{\theta} \nabla_{\boldsymbol{q}} \Phi \right) . \qquad (2.2.22)$$

The terms in equations (2.2.21) and (2.2.22) that do not involve gradients of g cancel in equation (2.2.20) to give

$$(\mathcal{L}_A f, g)_{\mathbb{H}} = - \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left[\nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} g - \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} g \right] \frac{f}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} = - (f, \mathcal{L}_A g)_{\mathbb{H}} \, . \qquad (2.2.23)$$

2.2.2 More Precise Statements

The formal calculations on symmetry and anti-symmetry will be made more rigorous in this section. The following material makes use of the necessary functional analysis theorems catalogued in appendix A.1. Certain parts of the calculations will remain formal. I will take special care to point out where this happens.

Lemma 2.2.2. *$\mathcal{L}_S$ is a densely defined self-adjoint operator on $\mathbb{H}$ with*

$$\operatorname{Dom}(\mathcal{L}_S) = \left\{ u \in \mathbb{H} \quad \Big| \quad \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left| \boldsymbol{\Lambda\Omega}\mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right|^2 \frac{1}{\mathcal{G}_o}\, d\boldsymbol{p}\, d\boldsymbol{q} < \infty \,, \right.$$
$$\left. \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left| \nabla_{\boldsymbol{p}} \cdot \left(\boldsymbol{\Xi}\mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right) \right|^2 \frac{1}{\mathcal{G}_o}\, d\boldsymbol{p}\, d\boldsymbol{q} < \infty \right\} . \tag{2.2.24}$$

Proof. I will use Theorem A.1.1 to prove that $\mathcal{L}_S$ is self-adjoint. Define

$$Gu = \sqrt{\theta}\boldsymbol{\Lambda\Omega}\mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \,, \tag{2.2.25}$$

with

$$\operatorname{Dom}(G) = \left\{ u \in \mathbb{H} \,\Big|\, \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left| \sqrt{\theta}\boldsymbol{\Lambda\Omega}\mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right|^2 \frac{1}{\mathcal{G}_o}\, d\boldsymbol{p}\, d\boldsymbol{q} < \infty \right\} . \tag{2.2.26}$$

Note that $C_o^\infty\left(\mathcal{Q} \times \mathbb{R}^N\right)$, the collection of smooth functions with compact support defined on $\mathcal{Q} \times \mathbb{R}^N$, is contained in $\operatorname{Dom}(G)$. Hence, $\operatorname{Dom}(G)$ is dense in $\mathbb{H}$. In fact this domain is the largest domain for which

$$\operatorname{Range}(G) \subset \mathbb{H}^N = \{(u_1, u_2, \ldots, u_N) \text{ where } u_i \in \mathbb{H}\, \forall\, i\} \,. \tag{2.2.27}$$

Also, at least on $\left(C_o^\infty\left(\mathcal{Q} \times \mathbb{R}^N\right)\right)^N$, a straightforward calculation shows

$$G^*\boldsymbol{v} = -\nabla_{\boldsymbol{p}} \cdot \left(\sqrt{\theta}\boldsymbol{\Omega}^T \boldsymbol{\Lambda v} \right) . \tag{2.2.28}$$

Now, by an easy modification of definition A.1.1,

$$\operatorname{Dom}(G^*) = \left\{ \boldsymbol{v} \in \mathbb{H}^N \,\big|\, \exists\, C \text{ s.t. } (\boldsymbol{v}, Gu)_{\mathbb{H}^N} \le C\, ||u||_{\mathbb{H}}\ \forall\, u \in \operatorname{Dom}(G) \right\} , \tag{2.2.29}$$

where

$$(\boldsymbol{v}, Gu)_{\mathbb{H}^N} = \left(\sum_{i=1}^N \left(v_i, (Gu)_i\right)_{\mathbb{H}} \right)^{1/2} . \tag{2.2.30}$$

Define

$$D^* = \left\{ \boldsymbol{v} \in \mathbb{H}^N \mid \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left| \nabla_{\boldsymbol{p}} \cdot \left(\sqrt{\theta} \boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v} \right) \right|^2 \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} < \infty \right\} . \tag{2.2.31}$$

Our first goal will be to show that, in fact, $\mathrm{Dom}\,(G^*) = D^*$. Note that it is clear that $\mathrm{Dom}\,(G^*) \subset D^*$ because $\mathrm{Dom}\,(G^*)$ is one of the sets on which $\mathrm{Range}\,(G^*) \subset \mathbb{H}^N$ and D^* is the largest of these. Hence, all that is left is to show $D^* \subset \mathrm{Dom}\,(G^*)$.

So, pick $\boldsymbol{v} \in D^*$ and consider

$$\begin{aligned} |(\boldsymbol{v}, Gu)_{\mathbb{H}^N}| &= \left| \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \boldsymbol{v} \cdot \left(\sqrt{\theta} \boldsymbol{\Lambda} \boldsymbol{\Omega} \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right) \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \right| \\ &= \left| \int\limits_{\mathcal{Q}} \int\limits_{B_R} \boldsymbol{v} \cdot \left(\sqrt{\theta} \boldsymbol{\Lambda} \boldsymbol{\Omega} \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right) \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \right. \\ &\qquad \left. + \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N \setminus B_R} \boldsymbol{v} \cdot \left(\sqrt{\theta} \boldsymbol{\Lambda} \boldsymbol{\Omega} \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right) \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \right| , \end{aligned} \tag{2.2.32}$$

where B_R is the ball of radius R in $\mathbb{R}^N$. Now the next step is formal, but the path to rigor is indicated in the discussion to follow. We write

$$\begin{aligned} &\int\limits_{\mathcal{Q}} \int\limits_{B_R} \boldsymbol{v} \cdot \left(\sqrt{\theta} \boldsymbol{\Lambda} \boldsymbol{\Omega} \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right) \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} \\ &= - \int\limits_{\mathcal{Q}} \int\limits_{B_R} \sqrt{\theta} \nabla_{\boldsymbol{p}} \cdot \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v} \right) \frac{u}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} + \int\limits_{\mathcal{Q}} \int\limits_{\partial B_R} \sqrt{\theta} \frac{u}{\mathcal{G}_o} \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v} \right) \cdot d\boldsymbol{n} \, d\boldsymbol{q} \, . \end{aligned} \tag{2.2.33}$$

This is a straightforward application of the Gauss-Green theorem (see [18]) only if u and $\boldsymbol{v}$ are smooth. In the current setting we are only assuming that $u \in \mathbb{H}$ and so it is not even clear that sense can be made of u on ∂B_R as this is a set of measure zero in $\mathbb{R}^N$. In order to make the above argument go through in the current setting we need to mimic the proof of the Trace Theorem (Theorem 1 in

Section 5.5 of [18]). The function u is mollified so that it is smooth near ∂B_R. The Gauss-Green theorem works on this mollified function and taking a limit as the mollification parameter approaches zero gives the result. Another application of the Gauss-Green theorem (using the fact that $\partial B_R = -\partial\left(\mathbb{R}^N \setminus B_R\right)$) yields

$$\int_{\mathcal{Q}} \int_{\partial B_R} \sqrt{\theta} \frac{u}{\mathcal{G}_o} \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \cdot d\boldsymbol{n}\, d\boldsymbol{q} = -\int_{\mathcal{Q}} \int_{\mathbb{R}^N \setminus B_R} \sqrt{\theta} \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \cdot \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o}\right) d\boldsymbol{p}\, d\boldsymbol{q} - \int_{\mathcal{Q}} \int_{\mathbb{R}^N \setminus B_R} \sqrt{\theta} \nabla_{\boldsymbol{p}} \cdot \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \frac{u}{\mathcal{G}_o} d\boldsymbol{p}\, d\boldsymbol{q}\,. \tag{2.2.34}$$

These manipulations lead to

$$\begin{aligned} \int_{\mathcal{Q}} \int_{B_R} \boldsymbol{v} \cdot \left(\sqrt{\theta} \boldsymbol{\Lambda} \boldsymbol{\Omega} \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o}\right)\right) \frac{1}{\mathcal{G}_o} d\boldsymbol{p}\, d\boldsymbol{q} & \\ = -\int_{\mathcal{Q}} \int_{B_R} \sqrt{\theta} \nabla_{\boldsymbol{p}} \cdot \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \frac{u}{\mathcal{G}_o} d\boldsymbol{p}\, d\boldsymbol{q} & \\ - \int_{\mathcal{Q}} \int_{\mathbb{R}^N \setminus B_R} \sqrt{\theta} \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \cdot \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o}\right) d\boldsymbol{p}\, d\boldsymbol{q} & \\ - \int_{\mathcal{Q}} \int_{\mathbb{R}^N \setminus B_R} \sqrt{\theta} \nabla_{\boldsymbol{p}} \cdot \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \frac{u}{\mathcal{G}_o} d\boldsymbol{p}\, d\boldsymbol{q}\,, & \end{aligned} \tag{2.2.35}$$

which we can insert into equation (2.2.32) to find

$$\begin{aligned} |(\boldsymbol{v}, Gu)| \leq & \left| \int_{\mathcal{Q}} \int_{B_R} \sqrt{\theta} \nabla_{\boldsymbol{p}} \cdot \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \frac{u}{\mathcal{G}_o} d\boldsymbol{p}\, d\boldsymbol{q} \right| \\ & + \left| \int_{\mathcal{Q}} \int_{\mathbb{R}^N \setminus B_R} \sqrt{\theta} \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \cdot \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o}\right) d\boldsymbol{p}\, d\boldsymbol{q} \right| \\ & + \left| \int_{\mathcal{Q}} \int_{\mathbb{R}^N \setminus B_R} \sqrt{\theta} \nabla_{\boldsymbol{p}} \cdot \left(\boldsymbol{\Omega}^T \boldsymbol{\Lambda} \boldsymbol{v}\right) \frac{u}{\mathcal{G}_o} d\boldsymbol{p}\, d\boldsymbol{q} \right| \\ & + \left| \int_{\mathcal{Q}} \int_{\mathbb{R}^N \setminus B_R} \boldsymbol{v} \cdot \left(\sqrt{\theta} \boldsymbol{\Lambda} \boldsymbol{\Omega} \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o}\right)\right) \frac{1}{\mathcal{G}_o} d\boldsymbol{p}\, d\boldsymbol{q} \right|. \end{aligned} \tag{2.2.36}$$

Two applications of the Cauchy-Schwarz inequality, one on the standard $\mathbb{R}^N$ inner product and one on the inner product in $\mathbb{H}$ gives

$$\begin{aligned}
&\int_{\mathcal{Q}}\int_{\mathbb{R}^N} \boldsymbol{v}\cdot \left(\sqrt{\theta}\boldsymbol{\Lambda}\boldsymbol{\Omega}\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{u}{\mathcal{G}_o}\right)\right)\frac{1}{\mathcal{G}_o}\,d\boldsymbol{p}\,d\boldsymbol{q} \\
&\qquad \le \int_{\mathcal{Q}}\int_{\mathbb{R}^N} |\boldsymbol{v}|\left|\sqrt{\theta}\boldsymbol{\Lambda}\boldsymbol{\Omega}\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{u}{\mathcal{G}_o}\right)\right|\frac{1}{\mathcal{G}_o}\,d\boldsymbol{p}\,d\boldsymbol{q} \\
&\qquad \le \left(\int_{\mathcal{Q}}\int_{\mathbb{R}^N} |\boldsymbol{v}|^2\frac{1}{\mathcal{G}_o}\,d\boldsymbol{p}\,d\boldsymbol{q}\right)^{1/2}\left(\int_{\mathcal{Q}}\int_{\mathbb{R}^N} \left|\sqrt{\theta}\boldsymbol{\Lambda}\boldsymbol{\Omega}\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{u}{\mathcal{G}_o}\right)\right|^2\frac{1}{\mathcal{G}_o}\,d\boldsymbol{p}\,d\boldsymbol{q}\right)^{1/2}.
\end{aligned} \tag{2.2.37}$$

Both factors in (2.2.37) are bounded, the first one because we are assuming $\boldsymbol{v} \in \mathbb{H}^N$, and the other because $u \in \mathrm{Dom}\,(G)$.

Similarly, because $\boldsymbol{v} \in D^*$ and $u \in \mathbb{H}$, we have

$$\begin{aligned}
&\left|\int_{\mathcal{Q}}\int_{\mathbb{R}^N} \sqrt{\theta}\nabla_{\boldsymbol{p}}\cdot\left(\boldsymbol{\Omega}^T\boldsymbol{\Lambda}\boldsymbol{v}\right)\frac{u}{\mathcal{G}_o}\,d\boldsymbol{p}\,d\boldsymbol{q}\right| \\
&\quad \le \left(\int_{\mathcal{Q}}\int_{\mathbb{R}^N} \left|\sqrt{\theta}\nabla_{\boldsymbol{p}}\cdot\left(\boldsymbol{\Omega}^T\boldsymbol{\Lambda}\boldsymbol{v}\right)\right|^2\frac{1}{\mathcal{G}_o}\,d\boldsymbol{p}\,d\boldsymbol{q}\right)^{1/2}\left(\int_{\mathcal{Q}}\int_{\mathbb{R}^N} |u|^2\frac{1}{\mathcal{G}_o}\,d\boldsymbol{p}\,d\boldsymbol{q}\right)^{1/2} < \infty\,.
\end{aligned} \tag{2.2.38}$$

These two integrals being bounded implies that we can take R to infinity in equation (2.2.36) and obtain

$$|(\boldsymbol{v}, Gu)_{\mathbb{H}^N}| \le \left|\int_{\mathcal{Q}}\int_{\mathbb{R}^N} \sqrt{\theta}\nabla_{\boldsymbol{p}}\cdot\left(\boldsymbol{\Omega}^T\boldsymbol{\Lambda}\boldsymbol{v}\right)\frac{u}{\mathcal{G}_o}\,d\boldsymbol{p}\,d\boldsymbol{q}\right|. \tag{2.2.39}$$

One final application of the Cauchy-Schwarz inequality gives the result and so $\mathrm{Dom}\,(G^*) = D^*$. Finally, we notice that

$$G^*G = -\mathcal{L}_S\,, \tag{2.2.40}$$

and so by Theorem A.1.1 we have that $\mathcal{L}_S$ is self-adjoint with domain given by

$$\begin{aligned}\operatorname{Dom}(\mathcal{L}_S) &= \operatorname{Dom}(G^*G) = \{u \in \operatorname{Dom}(G) \mid Gu \in \operatorname{Dom}(G^*)\} \\ &= \Bigg\{ u \in \mathbb{H} \,\Big|\, \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left| \sqrt{\theta} \boldsymbol{\Lambda} \boldsymbol{\Omega} \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right|^2 \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} < \infty \,, \\ &\qquad \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left| \nabla_{\boldsymbol{p}} \cdot \left(\boldsymbol{\Xi} \theta \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{u}{\mathcal{G}_o} \right) \right) \right|^2 \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} < \infty \Bigg\} . \end{aligned} \tag{2.2.41}$$

$\square$

Lemma 2.2.3. *$\mathcal{L}_A$ is a densely defined skew-adjoint operator on $\mathbb{H}$ with*

$$\operatorname{Dom}(\mathcal{L}_A) = \Bigg\{ u \in \mathbb{H} \,\Big|\, \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \left| \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} u + \mathbf{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} u \right|^2 \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p} \, d\boldsymbol{q} < \infty \Bigg\} . \tag{2.2.42}$$

We will further assume that $\int\limits_{\mathbb{R}^N} \int\limits_{\partial \mathcal{Q}} uv \frac{1}{\mathcal{G}_o} \mathbf{M}^{-1} \boldsymbol{p} \cdot d\boldsymbol{n} \, d\boldsymbol{p} = 0$ *for* $u, v \in \operatorname{Dom}(\mathcal{L}_A)$.

Proof. The proof of this lemma follows the same pattern as that of Lemma 2.2.2 with one minor difference. The key point is still to show that $\operatorname{Dom}(\mathcal{L}_A^*) = \operatorname{Dom}(-\mathcal{L}_A) = \operatorname{Dom}(\mathcal{L}_A)$ and this is done by demonstrating that the integration by parts used formally in equation (2.2.20) actually makes sense.

The $\nabla_{\boldsymbol{p}}$ term in $\mathcal{L}_A$ is treated exactly the same as in the proof of Lemma 2.2.2, there is just one small change in the $\nabla_{\boldsymbol{q}}$ term. The extra assumption in the lemma statement makes an appearance. In order to show that the integration by parts goes through we write (after some elementary rearrangement)

$$\begin{aligned}\int\limits_{\mathbb{R}^N} \int\limits_{\mathcal{Q}} \nabla_{\boldsymbol{q}} \cdot \left(u \boldsymbol{M}^{-1} \boldsymbol{p} \right) \frac{v}{\mathcal{G}_o} \, d\boldsymbol{q} &= - \int\limits_{\mathbb{R}^N} \int\limits_{\mathcal{Q}} u \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} \left(\frac{v}{\mathcal{G}_o} \right) \, d\boldsymbol{q} \, d\boldsymbol{p} \\ &\qquad + \int\limits_{\mathbb{R}^N} \int\limits_{\partial \mathcal{Q}} uv \frac{1}{\mathcal{G}_o} \boldsymbol{M}^{-1} \boldsymbol{p} \cdot d\boldsymbol{n} \, d\boldsymbol{p} \, . \end{aligned} \tag{2.2.43}$$

Once we add the extra assumption the rest of the proof goes through. $\square$

Remark 2.2.1. I believe the extra assumption here is unnecessary. It should follow directly from the formal assumption that the particles do not collide in finite time. After all, heuristically this means the allowable densities will integrate to zero on the "collision set" $\partial\mathcal{Q}$. The rigorous demonstration of this intuition is beyond the scope of the thesis.

Lemmas 2.2.2 and 2.2.3 together allow a statement about the operator $\mathcal{L}$ in

Lemma 2.2.4. *$\mathcal{L} = \mathcal{L}_A + \mathcal{L}_S$ is a densely defined operator on $\mathbb{H}$ with*

$$\mathrm{Dom}\left(\mathcal{L}\right) = \mathrm{Dom}\left(\mathcal{L}_A\right) \cap \mathrm{Dom}\left(\mathcal{L}_S\right) \,. \tag{2.2.44}$$

2.3 Relative Entropy Dissipation

In this section we define an entropy for our system. Recall the global equilibrium introduced in equation (2.2.16) rewritten here for convenience:

$$\mathcal{G}_o(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{\sqrt{\det\left(2\pi\theta \boldsymbol{M}\right)} Z_o} \exp\left(-\frac{1}{\theta}\left(\frac{1}{2}\boldsymbol{p}\cdot\boldsymbol{M}^{-1}\boldsymbol{p} + \varPhi\left(\boldsymbol{q}\right)\right)\right) \,. \tag{2.3.1}$$

Lemma 2.3.1. *Define*

$$\mathcal{H}\left[F; \mathcal{G}_o\right] = \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} F \log\left(\frac{F}{\mathcal{G}_o}\right) - F + \mathcal{G}_o \, d\boldsymbol{p}\, d\boldsymbol{q} \,, \tag{2.3.2}$$

the relative entropy of F with respect to $\mathcal{G}_o$. The full system dissipates the entropy given in equation (2.3.2), that is, $\frac{d}{dt}\mathcal{H}\left[F; \mathcal{G}_o\right] \leq 0$ for F solving the forward Kolmogorov equation (2.2.2)*.*

Proof. It is important to first address whether or not this integral makes sense. It is in fact true that for $F \in \mathbb{H}$ we must have $\mathcal{H}\left[F; \mathcal{G}_o\right] < \infty$. We show this by taking advantage of the elementary inequality

$$-1 \leq z \log z - z \leq z^2 \text{ whenever } z \geq 0 \,. \tag{2.3.3}$$

First note that this inequality is applicable since all the solutions we will be considering for equation (2.2.2) will be positive. This is assured since initial densities will be positive and solutions to such parabolic equations preserve positivity. This follows from the maximum principle, see for instance [30].

So, proceeding formally with this inequality we have

$$\begin{aligned}
0 &= -\int\limits_{\mathcal{Q}}\int\limits_{\mathbb{R}^N} \mathcal{G}_o \, d\boldsymbol{p}\, d\boldsymbol{q} + \int\limits_{\mathcal{Q}}\int\limits_{\mathbb{R}^N} \mathcal{G}_o \, d\boldsymbol{p}\, d\boldsymbol{q} \\
&\leq \mathcal{H}\left[F;\mathcal{G}_o\right] = \int\limits_{\mathcal{Q}}\int\limits_{\mathbb{R}^N} \left[\frac{F}{\mathcal{G}_o}\log\left(\frac{F}{\mathcal{G}_o}\right) - \frac{F}{\mathcal{G}_o}\right]\mathcal{G}_o \, d\boldsymbol{p}\, d\boldsymbol{q} + \int\limits_{\mathcal{Q}}\int\limits_{\mathbb{R}^N} \mathcal{G}_o \, d\boldsymbol{p}\, d\boldsymbol{q} \\
&\leq \int\limits_{\mathcal{Q}}\int\limits_{\mathbb{R}^N} F^2 \frac{1}{\mathcal{G}_o} \, d\boldsymbol{p}\, d\boldsymbol{q} + 1 < \infty\,,
\end{aligned} \tag{2.3.4}$$

which shows that $\mathcal{H}$ is well-defined on $\mathbb{H}$.

We begin by showing that it satisfies a local dissipation law. Global dissipation follows immediately (formally).

Define

$$h\left(F\right) = F\log\left(\frac{F}{\mathcal{G}_o}\right) - F + \mathcal{G}_o\,, \tag{2.3.5}$$

and note that

$$\partial_t h = \partial_t F \log\left(\frac{F}{\mathcal{G}_o}\right) . \tag{2.3.6}$$

Assuming F solves the forward Kolmogorov equation (2.2.2) we have

$$\begin{aligned}
&\partial_t h + \log\left(\frac{F}{\mathcal{G}_o}\right)\boldsymbol{M}^{-1}\boldsymbol{p}\cdot\nabla_{\boldsymbol{q}}F - \log\left(\frac{F}{\mathcal{G}_o}\right)\nabla_{\boldsymbol{q}}\Phi\cdot\nabla_{\boldsymbol{p}}F \\
&\qquad = \log\left(\frac{F}{\mathcal{G}_o}\right)\nabla_{\boldsymbol{p}}\cdot\left[\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right)\right] .
\end{aligned} \tag{2.3.7}$$

The identities below help us establish the result:

$$\nabla_{\boldsymbol{q}} \cdot \left(\boldsymbol{M}^{-1} \boldsymbol{p} F \log \left(\frac{F}{\mathcal{G}_o} \right) \right) = \log \left(\frac{F}{\mathcal{G}_o} \right) \nabla_{\boldsymbol{q}} \cdot \left(\boldsymbol{M}^{-1} \boldsymbol{p} F \right) + \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} \left(\frac{F}{\mathcal{G}_o} \right) \mathcal{G}_o \,, \tag{2.3.8}$$

$$\nabla_{\boldsymbol{p}} \cdot \left(\nabla_{\boldsymbol{q}} \Phi F \log \left(\frac{F}{\mathcal{G}_o} \right) \right) = \log \left(\frac{F}{\mathcal{G}_o} \right) \nabla_{\boldsymbol{p}} \cdot \left(\nabla_{\boldsymbol{q}} \Phi F \right) + \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} \left(\frac{F}{\mathcal{G}_o} \right) \mathcal{G}_o \,. \tag{2.3.9}$$

These imply

$$\begin{aligned} &\log \left(\frac{F}{\mathcal{G}_o} \right) \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} F - \log \left(\frac{F}{\mathcal{G}_o} \right) \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} F \\ &\qquad = \nabla_{\boldsymbol{q}} \cdot \left(\boldsymbol{M}^{-1} \boldsymbol{p} F \log \left(\frac{F}{\mathcal{G}_o} \right) \right) - \nabla_{\boldsymbol{p}} \cdot \left(\nabla_{\boldsymbol{q}} \Phi F \log \left(\frac{F}{\mathcal{G}_o} \right) \right) \\ &\qquad\qquad + \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} \left(\frac{F}{\mathcal{G}_o} \right) \mathcal{G}_o - \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} \left(\frac{F}{\mathcal{G}_o} \right) \mathcal{G}_o \,. \end{aligned} \tag{2.3.10}$$

Now look at the last two terms in this equation

$$\begin{aligned} &\nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} \left(\frac{F}{\mathcal{G}_o} \right) \mathcal{G}_o - \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} \left(\frac{F}{\mathcal{G}_o} \right) \mathcal{G}_o \\ &\qquad = \nabla_{\boldsymbol{q}} \Phi \cdot \left(\frac{\mathcal{G}_o \nabla_{\boldsymbol{p}} F - F \nabla_{\boldsymbol{p}} \mathcal{G}_o}{\mathcal{G}_o^2} \right) \mathcal{G}_o - \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \left(\frac{\mathcal{G}_o \nabla_{\boldsymbol{q}} F - F \nabla_{\boldsymbol{q}} \mathcal{G}_o}{\mathcal{G}_o^2} \right) \mathcal{G}_o \\ &\qquad = \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} F - \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} F + \frac{F}{\mathcal{G}_o} \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} \mathcal{G}_o - \frac{F}{\mathcal{G}_o} \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} \mathcal{G}_o \\ &\qquad = \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} F - \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} F \cancel{- \frac{1}{\theta} F \boldsymbol{M}^{-1} \boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} \Phi} + \cancel{\frac{1}{\theta} F \nabla_{\boldsymbol{q}} \Phi \cdot \boldsymbol{M}^{-1} \boldsymbol{p}} \\ &\qquad = \nabla_{\boldsymbol{p}} \cdot \left(F \nabla_{\boldsymbol{q}} \Phi \right) - \nabla_{\boldsymbol{q}} \cdot \left(F \boldsymbol{M}^{-1} \boldsymbol{p} \right) \,. \end{aligned} \tag{2.3.11}$$

By combining these we have

$$\begin{aligned} &\partial_t h + \nabla_{\boldsymbol{q}} \cdot \left[\left(F \log \left(\frac{F}{\mathcal{G}_o} \right) - F \right) \boldsymbol{M}^{-1} \boldsymbol{p} \right] - \nabla_{\boldsymbol{p}} \cdot \left[\left(F \log \left(\frac{F}{\mathcal{G}_o} \right) - F \right) \nabla_{\boldsymbol{q}} \Phi \right] \\ &\qquad = \log \left(\frac{F}{\mathcal{G}_o} \right) \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi} \theta \mathcal{G}_o \nabla_{\boldsymbol{p}} \left(\frac{F}{\mathcal{G}_o} \right) \right] \,. \end{aligned} \tag{2.3.12}$$

Note that by adding and subtracting $\mathcal{G}_o$ in the correct place and cancelling we can write

$$\partial_t h + \nabla_{\boldsymbol{q}} \cdot \left(h\boldsymbol{M}^{-1}\boldsymbol{p}\right) - \nabla_{\boldsymbol{p}} \cdot \left(h\nabla_{\boldsymbol{q}}\Phi\right) = \log\left(\frac{F}{\mathcal{G}_o}\right)\nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right)\right] . \tag{2.3.13}$$

Now we tackle the right-hand side:

$$\begin{aligned}
&\log\left(\frac{F}{\mathcal{G}_o}\right)\nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right)\right] \\
&\qquad = \nabla_{\boldsymbol{p}} \cdot \left[\log\left(\frac{F}{\mathcal{G}_o}\right)\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right)\right] - \frac{\mathcal{G}_o^2}{F}\theta\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right) \cdot \boldsymbol{\Xi}\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right) .
\end{aligned} \tag{2.3.14}$$

All together we have

$$\begin{aligned}
\partial_t h + \nabla_{\boldsymbol{q}} \cdot \left(h\boldsymbol{M}^{-1}\boldsymbol{p}\right) - \nabla_{\boldsymbol{p}} \cdot \left(h\nabla_{\boldsymbol{q}}\Phi\right) - \nabla_{\boldsymbol{p}} \cdot \left[\log\left(\frac{F}{\mathcal{G}_o}\right)\boldsymbol{\Xi}\theta\mathcal{G}_o\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right)\right] \\
= -\frac{\mathcal{G}_o^2}{F}\theta\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right) \cdot \boldsymbol{\Xi}\nabla_{\boldsymbol{p}}\left(\frac{F}{\mathcal{G}_o}\right) .
\end{aligned} \tag{2.3.15}$$

Now, referring to the properties of $\boldsymbol{\Xi}$ discussed in Section A.4 we know that the right-hand side is non-positive. More can be said in fact. In the simplest case we know the smallest nonzero eigenvalue of $\boldsymbol{\Xi}$ and it should be possible to get an estimate for the smallest nonzero eigenvalue in the general case once we know more about the form of $\boldsymbol{\Lambda}$. This is beyond the scope of this thesis.

For now we simply note that

$$\frac{d}{dt}\mathcal{H}\left[F;\mathcal{G}_o\right] = \int\limits_{\mathcal{Q}}\int\limits_{\mathbb{R}^N} \partial_t h \, d\boldsymbol{p} \, d\boldsymbol{q} \leq 0 \,, \tag{2.3.16}$$

since the integral of the divergence term is 0 for $h \in \mathrm{Dom}\left(\mathcal{L}\right) \subset \mathbb{H}$. This formally obvious fact is justified just as in the proof of the Lemmas 2.2.2 and 2.2.3. $\square$

Chapter 3

Modified Zwanzig-Mori Formalism

In this chapter I will describe the new formalism, beginning with a very brief overview of Zwanzig's work. Following the brief summary of the basic ideas of the Zwanzig-Mori formalism I will introduce recent uses and clarifications of it. This will lead to the heart of our modification: the idea of a hierarchy of models related to one another by Zwanzig-Mori projections. The remainder of the chapter will be used to investigate formally the low-energy limit for our model in this context. In particular, we will follow ideas put forward by Chorin [6,8–14], Goldenfeld [2–5, 22–24], and others and introduce a renormalization map. It will become apparent that to understand the hierarchy we will need to take a hydrodynamic limit which will be the topic for the last two chapters of the thesis.

3.1 Zwanzig and Mori's Idea

In the 60s and 70s Zwanzig [35–37] and Mori [28] presented a framework for studying out-of-equilibrium systems. In this section I will outline in broad terms the idea presented in [36] by Zwanzig. I will describe the heart of his idea via its use by Chorin and collaborators [1, 6, 8–14]. In particular, I will follow the presentation in [14]. I will also describe a particular way of framing the formalism presented by E and Engquist [16].

3.1.1 Broad Outline of the Problem

Consider a large collection of point particles moving under some potential V in free space. The i^{th} particle has mass m_i, momentum $\boldsymbol{p}_i$ and position $\boldsymbol{q}_i$. The Hamiltonian H for the system is

$$H\left(\vec{\boldsymbol{p}}, \vec{\boldsymbol{q}}\right) = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i \cdot \boldsymbol{p}_i}{2m_i} + V(\boldsymbol{q}_1, \boldsymbol{q}_2, ..., \boldsymbol{q}_N)\,, \tag{3.1.1}$$

where $\vec{\boldsymbol{q}} = (\boldsymbol{q}_1, \boldsymbol{q}_2, ..., \boldsymbol{q}_N)$ and $\vec{\boldsymbol{p}} = (\boldsymbol{p}_1, \boldsymbol{p}_2, ..., \boldsymbol{p}_N)$. Note that a slight change of notation has been made. Now, with $\phi = (\vec{\boldsymbol{p}}, \vec{\boldsymbol{q}}) \in \mathbb{R}^{6N}$ we can describe the precise time evolution of the N-particle system by Hamilton's equations of motion:

$$\dot{\phi} = \boldsymbol{J}\nabla H\left(\phi\right) := R(\phi)\,, \tag{3.1.2}$$

$$\boldsymbol{J} = \begin{pmatrix} \boldsymbol{0} & \boldsymbol{I} \\ -\boldsymbol{I} & \boldsymbol{0} \end{pmatrix}.$$

For any realistic system N is so large that numerical solution is impossible (e.g. for the air in a room $N \approx 10^{23}$) even if the initial condition for every molecule could be determined; hence, the obvious need for a reduced system.

3.1.2 Associated Liouville Equation

What I present here is just a partial outline of Zwanzig's work followed by a particular example drawn from Chorin and Stinis [14].

First, let $f : \mathbb{R}^{6N} \times [0, \infty) \to \mathbb{R}$ be the phase space density corresponding to the dynamics $\dot{\phi} = R(\phi)$. It is well known [18] that f satisfies the Liouville equation[1]

$$\partial_t f = \mathcal{L}_L f \,, \tag{3.1.3}$$

$$f(x,0) = f_0(x) \text{ (the initial density)} \,, \tag{3.1.4}$$

where

$$\mathcal{L}_L f = -\nabla \cdot (fR) \,.$$

The linear, first-order partial differential equation (3.1.3) is the real starting point for Zwanzig's derivations. Note that this change of setting from a huge collection of nonlinear ordinary differential equations to a single linear partial differential equation is not as helpful as the attributes of the equations might suggest. The partial differential equation is defined on $\mathbb{R}^{6N} \times [0,\infty)$ and no easier to solve. Further reduction is required. Zwanzig provides a recipe for reducing the order of (3.1.3). In the next subsection I will describe the reduction.

3.1.3 Zwanzig's Formal Argument

The following manipulations are drawn in spirit from Zwanzig's 1960 work [35]. I have only simplified his notation by a small amount. First introduce an operator $\mathbb{P} : \mathcal{D}\left(\mathbb{R}^{6N}\right) \to \mathcal{D}\left(\mathbb{R}^{6N}\right)$ where $\mathcal{D}\left(\mathbb{R}^{6N}\right)$ is the collection of distributions on $\mathbb{R}^{6N}$. Require that $\mathbb{P}$ have the following properties:

1. linearity

2. time independent

[1] Alternatively we could consider the problem from the reverse perspective: that is, we could view the ordinary differential equation (3.1.2) as describing the characteristics for the Liouville equation.

3. $\mathbb{P}^2 = \mathbb{P}$ (i.e. $\mathbb{P}$ must be a projection)

The idea is that we will find some $\mathbb{P}$ that will reduce the order of equation 3.1.3. The above properties are the natural ones to ask for. Now, let $f_1 = \mathbb{P}f$ and $f_2 = (\mathbb{I} - \mathbb{P}) f$ so that $f = f_1 + f_2$ where we interpret f_1 as the resolved or important part and f_2 is the remainder. Equation 3.1.3 becomes

$$\partial_t f_1 = \mathbb{P}\mathcal{L}_L f_1 + \mathbb{P}\mathcal{L}_L f_2, \tag{3.1.5}$$

$$\partial_t f_2 = (\mathbb{I} - \mathbb{P})\, \mathcal{L}_L f_2 + (\mathbb{I} - \mathbb{P})\, \mathcal{L}_L f_1\,. \tag{3.1.6}$$

Formally, we may solve (3.1.6) by introducing the semigroup notation (see Chapter 11 of [32] for an excellent discussion) and applying the variation of parameters method [32]. We find

$$f_2(t) = e^{t(\mathbb{I}-\mathbb{P})\mathcal{L}_L} f_2(0) + \int_0^t e^{s(\mathbb{I}-\mathbb{P})\mathcal{L}_L} (\mathbb{I} - \mathbb{P})\, \mathcal{L}_L f_1(t-s)ds\,, \tag{3.1.7}$$

and substitute this back into 3.1.5 to obtain

$$\begin{aligned} \frac{\partial f_1}{\partial t} = \mathbb{P}\mathcal{L}_L f_1 &+ \int_0^t \mathbb{P}\mathcal{L}_L e^{s(\mathbb{I}-\mathbb{P})\mathcal{L}_L} (\mathbb{I} - \mathbb{P})\, \mathcal{L}_L f_1(t-s)ds \\ &+ \mathbb{P}\mathcal{L}_L e^{t(\mathbb{I}-\mathbb{P})\mathcal{L}_L} f_2(0)\,. \end{aligned} \tag{3.1.8}$$

Remark 3.1.1. Equation (3.1.8) forms the basis for the so-called "fluctuation-dissipation" theorems in irreversible statistical mechanics. Chapter 6 of [7] includes a clear discussion of this connection.

To go beyond this general setup I will move away from Zwanzig's original work and follow the presentation of Chorin and Stinis [14]. They consider system (3.1.2) with an additional construct. Suppose one is only interested in the first m components of ϕ (after suitable reordering). This implies $\phi = \left(\widehat{\phi}, \widetilde{\phi}\right)$ where $\widehat{\phi} \in \mathbb{R}^m$ is the part we are interested in and $\widetilde{\phi} \in \mathbb{R}^{N-m}$ is the unknown or inaccessible part. One then further supposes that the system has an invariant density

$$f_{\mathrm{inv}}(\phi) = \frac{1}{Z} e^{-H(\phi)} . \tag{3.1.9}$$

The Zwanzig-Mori formalism is applied by defining a projection onto functions of $\widehat{\phi}$. They select the element of that set that is closest in the mean-square sense with respect to the invariant density, that is, by using the conditional expectation:

$$\mathbb{P}\left[R\right](\widehat{\phi}) = E\left[R(\phi)\middle|\widehat{\phi}\right] . \tag{3.1.10}$$

Note that this is an orthogonal projection onto the functions of $\widehat{\phi}$ with respect to the inner product

$$(u, v) = E\left[uv\right] = \int u(\phi)v(\phi)f_{\mathrm{inv}}(\phi)\, d\phi . \tag{3.1.11}$$

The connection to the renormalization group is made by showing that directly approximating equation (3.1.2) as

$$\frac{d}{dt}\widehat{\phi}(t) = E\left[R(\phi(t))\middle|\widehat{\phi}(t)\right] , \tag{3.1.12}$$

gives a new system that is also Hamiltonian with

$$\widehat{H}(\widehat{\phi}) = -\log \int \exp(-H(\widehat{\phi}, \widetilde{\phi}))\, d\widetilde{\phi} . \tag{3.1.13}$$

They also note that the new system has an invariant density given by $\widehat{f}_{\mathrm{inv}} = \widehat{Z}^{-1}\exp(-\widehat{H})$. This map $H \mapsto \widehat{H}$ is a renormalization group transformation. The work focuses on using the Zwanzig-Mori formalism to interpret[2] and propose various corrections to equation (3.1.12).

[2]It is not clear what relation the solution $\widehat{\phi}$ to (3.1.12) has to the full solution ϕ.

3.2 Heterogeneous Multiscale Methods

In 2003 Weinan E and Bjorn Engquist presented a general methodology for "the efficient numerical computation of problems with multi-scales and multi-physics, on multi-grids." [16] They note that for inherently multi-scale problems the standard approach has been to pick a scale you are interested in and eliminate all others by using a tool from the menagerie.[3] They argue that the relative weakness of these ideas in the setting of many complex systems is caused by the fact that we are often forced to introduce empirical closures that are "not always justified or understood."

Their work represents a synthesis for the purpose of simulation of a new approach: the so-called "first principles" approach. The main thrust of this collection of ideas has been to model the parameters of the macro-scale model directly on a micro-scale model, eliminating the need for additional empirical modeling. The piece of their work that is most important for us is their general framework. They separate the micro- and macro-scale processes into different state variables defined on different spaces and then connect them with compression and reconstruction operators. In the next section I will use this idea to describe our new formalism.

[3] They cite averaging methods in classical mechanics, homogenization theory, equilibrium statistical mechanics, WKB methods, nonequilibrium thermodynamics, kinetic theory, transition state theory, and turbulence models.

3.3 Modification of the Formalism

We follow [16] and define maps between densities on some large N-dimensional space to densities on some smaller n-dimensional space

$$\text{(compression map) } \mathbb{M} : \mathcal{D}\left(\mathbb{R}^N\right) \to \mathcal{D}\left(\mathbb{R}^n\right) \,, \tag{3.3.1}$$

$$\text{(reconstruction map) } \mathbb{E} : \mathcal{D}\left(\mathbb{R}^n\right) \to \mathcal{D}\left(\mathbb{R}^N\right) \,. \tag{3.3.2}$$

It is important to note that the domain and range for these maps will not be so simple for a real problem. The definition here is just for convenience. The maps $\mathbb{M}$ and $\mathbb{E}$ should be chosen so that $\mathbb{ME} = \mathbb{I}$. Then the projection operator $\mathbb{P} = \mathbb{EM}$ captures the important part of the system. The complimentary projection $\widetilde{\mathbb{P}} = \mathbb{I} - \mathbb{P}$ then captures the scales we want to ignore. In general we will be applying these maps to the domain of an operator $\mathcal{L}$ so that we may study equations like

$$\partial_t F = \mathcal{L} F \,. \tag{3.3.3}$$

This is intentionally vague. For the purposes of this thesis we will imagine $\mathcal{L}$ as either a Liouville operator or a forward Kolmogorov operator.

We decompose (3.3.3) into two equations for $F^{(1)} = \mathbb{P}F$ (the resolved part) and $\widetilde{F}^{(1)} = \widetilde{\mathbb{P}}F$ (the unresolved part)

$$\partial_t F^{(1)} = \mathbb{P}\mathcal{L}\mathbb{P}F^{(1)} + \mathbb{P}\mathcal{L}\widetilde{\mathbb{P}}\widetilde{F}^{(1)} \,, \tag{3.3.4}$$

$$\partial_t \widetilde{F}^{(1)} = \widetilde{\mathbb{P}}\mathcal{L}\mathbb{P}F^{(1)} + \widetilde{\mathbb{P}}\mathcal{L}\widetilde{\mathbb{P}}\widetilde{F}^{(1)} \,. \tag{3.3.5}$$

Now an approximation procedure is applied to obtain an expression for $\widetilde{F}^{(1)}$ in terms of $F^{(1)}$. For instance the Galerkin approximation (for correct choice of $\mathbb{E}$ and $\mathbb{M}$) corresponds to setting $\widetilde{F}^{(1)} \equiv 0$. Supposing $\mathcal{L}$ were a Liouville operator I conjecture that some nontrivial approximation for $\widetilde{F}^{(1)}$ will create a new partial differential equation that can be, in certain circumstances, interpreted as a Kolmogorov equation. This construction is beyond the scope of this thesis but it is a promising direction for future work since it would be a justification for considering stochastic systems to begin with.

After this approximation procedure one has

$$\partial_t F^{(1)} = \mathcal{L}^{(1)} F^{(1)} \,,$$

where $\mathcal{L}^{(1)}$ is some new linear (possibly non-local) operator. Repetition of this procedure produces a hierarchy of models and a map from one element of the hierarchy to another:

$$\left(F^{(i)}, \mathcal{L}^{(i)}\right) \mapsto \left(F^{(i+1)}, \mathcal{L}^{(i+1)}\right) .$$

As $N \to \infty$ this hierarchy becomes infinite. We term this formal procedure the modified Zwanzig-Mori formalism.

3.4 Future of the Modified Formalism

As motivation for what is to follow and as a general hope for the future I will describe the long-term goal for this formalism. The map between elements of the hierarchy above is similar in spirit to the renormalization group used by physicists. In that community the map is on coupling constants: one takes a system at a given level of detail and clumps the independent elements together by some rule and then rephrases the new system in the old form with new constants. In our setting we are simply replacing the coupling constants with the operator associated to the dynamics on phase space densities.

And, just as is done in renormalization group applications, we intend to seek a fixed point for the map on elements of hierarchy. This fixed point, and more importantly the linearization of the map at the fixed point, should give insight into the connection between scales in a problem. We have made modest steps in this direction.

3.5 Application to a Toy Model

As a first step we need to move a little away from the description of the formalism above. Instead of dealing with the hierarchy induced by considering $\mathbb{P} = \mathbb{E}\mathbb{M}$ which maps systems on $\mathbb{R}^N$ to systems on the same space, we want to consider just the compression part $\mathbb{M}$ of the map. I will define a reconstruction operator but will not make use of it in this thesis. This move to a smaller piece of the formalism is justified after the fact. That is: this is what I have tried and found to work, so it must have been the right thing to try.

3.5.1 Map Definitions

A critical component of our approach is that we make the compression and reconstruction maps dependent upon an "averaging map" A:

Definition 3.5.1. *(The Averaging Map) $A : \mathcal{M}^N \to \mathcal{M}^{N/m}$ A linear map from an N-dimensional manifold to an N/m-dimensional manifold.*

$$A(x_1, x_2, \ldots, x_N) = \left(\frac{x_1 + \cdots + x_m}{m}, \frac{x_{m+1} + \cdots + x_{2m}}{m}, \ldots, \frac{x_{N-m+1} + \cdots + x_N}{m} \right), \quad (3.5.1)$$

where $(x_1, x_2, \ldots, x_N) \in \mathcal{M}^N$ is a placeholder for a vector of positions or momenta.

Using the averaging map A we define the compression and reconstruction maps as follows.

Definition 3.5.2. *(The Compression Map) Let $\mathbb{H}_N$ denote the Hilbert space corresponding to an underlying N-particle model and define $\mathbb{M} : \mathbb{H}_N \to \mathbb{H}_{N/m}$ as*

$$\mathbb{M}\left[f\right](\bar{\boldsymbol{p}}, \bar{\boldsymbol{q}}) = \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \delta\left(\bar{\boldsymbol{p}} - A\boldsymbol{p}\right) \delta\left(\bar{\boldsymbol{q}} - A\boldsymbol{q}\right) f(\boldsymbol{p}, \boldsymbol{q})\, d\boldsymbol{p}\, d\boldsymbol{q}\,. \tag{3.5.2}$$

Definition 3.5.3. *(The Reconstruction Map) $\mathbb{E} : \mathbb{H}_{N/m} \to \mathbb{H}_N$*

Let $g \in \mathbb{H}_{N/m}$. We define $\mathbb{E}g$ as satisfying the constrained relative entropy minimization problem

$$\begin{aligned} S\left(\mathbb{E}g|\mathcal{G}_o\right) &= \int_{\mathbb{R}^{2N}} \mathbb{E}g \log\left(\frac{\mathbb{E}g}{\mathcal{G}_o}\right) dX \\ &= \min\left\{ S\left(U|\mathcal{G}_o\right) : \mathbb{M}U = g, \int_{\mathbb{R}^{2N}} U\, dX = 1 \right\}. \end{aligned} \tag{3.5.3}$$

Solving this minimization problem gives $\mathbb{E}g\left(X\right) = \frac{g(A(X))}{\mathbb{M}[\mathcal{G}_o](A(X))} \mathcal{G}_o\left(X\right)$.

Remark 3.5.1. The reconstruction map gives a density $\mathbb{E}g$ on the large space that is "close to the equilibrium density" while still pushing forward under compression to g.

3.5.2 Construction of Toy Model

We assume that the energy of the necklace is small and the mass of the particles is constant, so that $m_i = m_o$ for all i. Separating the potential energy part Φ out we have

$$\Phi\left(\boldsymbol{q}\right) = K \sum_{i=1}^{N-1} \frac{1}{\left(q_{i+1} - q_i\right)^p} + \frac{1}{\left(1 - \left(q_N - q_1\right)\right)^p}\,. \tag{3.5.4}$$

Φ has a minimum on the set $\left\{\left(0, \frac{1}{N}, \ldots, \frac{N-1}{N}\right) + \lambda\left(1, 1, \ldots, 1\right) \mid \lambda \in \mathbb{R}\right\}$; the collection of equi-distributed configurations. Calculating the Hessian of Φ on this set and removing the constant minimum from the Hamiltonian we have the low-energy Hamiltonian (in vector notation for ease of reading):

$$H \approx H_{LE} = \frac{1}{2m_o}\boldsymbol{p}\cdot\boldsymbol{p} + \frac{1}{2}K_N\left(\boldsymbol{q}-\mathbf{s}\right)\cdot\mathbf{Q}\left(\boldsymbol{q}-\mathbf{s}\right)\,, \tag{3.5.5}$$

where $K_N = Kp(p+1)N^{p+2}$,

$$\mathbf{Q} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & \ddots & 0 & 0 \\ 0 & -1 & 2 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ -1 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix}, \tag{3.5.6}$$

and $\mathbf{s} = \left(0, \frac{1}{N}, \ldots, \frac{N-1}{N}\right)$ is a generator of the minimum set for $\varPhi$.

Following formally the argument in Section 2.2.1 the Hamiltonian of our system implies the equilibrium density also has a simple form

$$F_{eq} = \frac{1}{\sqrt{\left(2\pi\theta m_o\right)^N}}\frac{1}{Z}\exp\left(-\frac{1}{\theta}\left(\frac{1}{2m_o}\boldsymbol{p}\cdot\boldsymbol{p} + \frac{1}{2}K_N(\boldsymbol{q}-\mathbf{s})\cdot\mathbf{Q}(\boldsymbol{q}-\mathbf{s})\right)\right)\,. \tag{3.5.7}$$

To apply the compression operator to this system we will need the following

Lemma 3.5.1. *(Handy Formal Trick)*

$$\mathbb{M}\left[\frac{\exp\left(-\frac{1}{2}X^TBX\right)}{\sqrt{\det\left(2\pi B^{-1}\right)}}\right] = \frac{\exp\left(-\frac{1}{2}x^T\left(AB^{-1}A^T\right)^{-1}x\right)}{\sqrt{\det\left(2\pi AB^{-1}A^T\right)}}\,. \tag{3.5.8}$$

Sketch of Proof.

$$\mathbb{M}\left[\frac{\exp\left(-\frac{1}{2}X^TBX\right)}{\sqrt{\det\left(2\pi B^{-1}\right)}}\right] = \frac{1}{\sqrt{\det\left(2\pi B^{-1}\right)}}\int\limits_{\mathbb{R}^N}\delta\left(x-AX\right)\exp\left(-\frac{1}{2}X^TBX\right)\,dX \tag{3.5.9}$$

is the distribution that maps $\psi \in C_o^\infty\left(\mathbb{R}^{N/m}\right)$ in the following way

$$\psi \mapsto \frac{1}{\sqrt{\det\left(2\pi B^{-1}\right)}} \int\limits_{\mathbb{R}^N} \psi\left(AX\right) \exp\left(-\tfrac{1}{2} X^T B X\right)\, dX\,. \tag{3.5.10}$$

Note that in order for this integral to make sense for general ψ we need that $A : N(B) \to 0$ which happens if and only if $N(A) \supset N(B)$. Proceeding formally, making use of Lemma A.2.1 we have

$$\begin{aligned}\frac{1}{\sqrt{\det\left(2\pi B^{-1}\right)}} &\int\limits_{\mathbb{R}^N} \psi\left(AX\right) \exp\left(-\tfrac{1}{2} X^T B X\right)\, dX \\ &= \exp\left(\tfrac{1}{2}\nabla_X^T B^{-1} \nabla_X\right) \psi\left(AX\right)\Bigg|_{X=0}\,.\end{aligned} \tag{3.5.11}$$

Now note that $\nabla_X = A^T \nabla_x$ so we have

$$\begin{aligned}\frac{1}{\sqrt{\det\left(2\pi B^{-1}\right)}} &\int\limits_{\mathbb{R}^N} \psi\left(AX\right) \exp\left(-\tfrac{1}{2} X^T B X\right)\, dX \\ &= \exp\left(\tfrac{1}{2}\nabla_x^T A B^{-1} A^T \nabla_x\right) \psi(x)\Bigg|_{x=0}\,.\end{aligned} \tag{3.5.12}$$

Applying Lemma A.2.1 again we see

$$\begin{aligned}\frac{1}{\sqrt{\det\left(2\pi B^{-1}\right)}} &\int\limits_{\mathbb{R}^N} \psi\left(AX\right) \exp\left(-\tfrac{1}{2} X^T B X\right)\, dX \\ = \frac{1}{\sqrt{\det\left(2\pi A B^{-1} A^T\right)}} &\int\limits_{\mathbb{R}^{N/m}} \psi(x) \exp\left(-\tfrac{1}{2} x^T \left(A B^{-1} A^T\right)^{-1} x\right)\, dx\,.\end{aligned} \tag{3.5.13}$$

This establishes the lemma. □

Now we apply the compression operator 3.5.2. Using the fact that

$$A A^T = \frac{1}{m}\boldsymbol{I}\,, \tag{3.5.14}$$

we have

$$
\begin{aligned}
&\mathbb{M}\left[F_{eq}\right](\bar{\boldsymbol{p}}, \bar{\boldsymbol{q}}) = f_{eq} \\
&= \frac{1}{Z_{new}} \exp\left(-\frac{1}{\theta}\left(\frac{1}{2(m_o/m)}\bar{\boldsymbol{p}} \cdot \bar{\boldsymbol{p}} + \frac{1}{2}K_N\left(\bar{\boldsymbol{q}} - \bar{\mathbf{s}}\right) \cdot \left(A\mathbf{Q}^{-1}A^T\right)^{-1}\left(\bar{\boldsymbol{q}} - \bar{\mathbf{s}}\right)\right)\right) .
\end{aligned}
\tag{3.5.15}
$$

3.5.3 Discussion of Toy Model Results

The important lesson is that the map on densities can be regarded as a map on particle systems. The new equilibrium is the equilibrium associated with an N/m-"parcel" system with coupling constants changed according to

$$
m_o \mapsto \frac{m_o}{m} , \tag{3.5.16}
$$

$$
K_N\mathbf{Q} \mapsto K_N\left(A\mathbf{Q}^{-1}A^T\right)^{-1} . \tag{3.5.17}
$$

This notion is enough to motivate the remainder of the thesis. We have a way of moving between an N particle model and an N/m parcel model via the compression operator. It should be clear that naively repeating this procedure will leave us with a trivial system. The route to removing this difficulty is *not* through the reconstruction operator. That map will be of help when we need to compare answers between a reduced model and the original. However, in this case it will not recover the information we have averaged out by compressing to a parcel model. The solution is to compare like objects. We need a mechanism for taking an N particle system and inflating it to an Nm particle model and then compressing that. Figure 3.1 is intended to hint at this situation.

One way to obtain a mechanism for model inflation is to imagine the particles

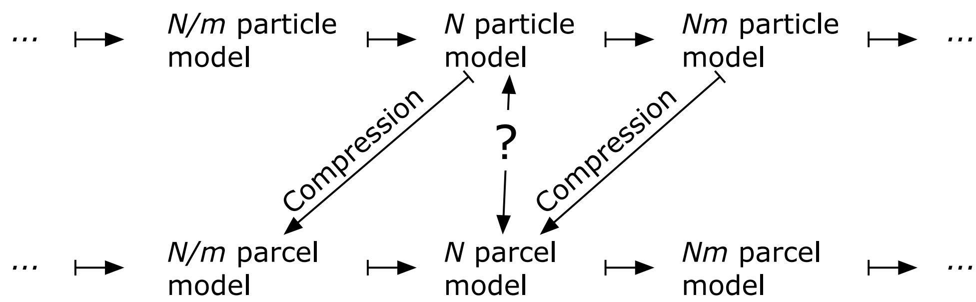

Figure 3.1: The compression map induces a map on particle systems. In order to have a meaningful fixed point for the modified Zwanzig-Mori formalism we need to examine the relation between N particle models and N parcel models.

as being the basis for an approximation of a density in the sense that

$$\sum_{i=1}^{N} m_i \delta(x - q_i) \sim \rho(x)\,. \tag{3.5.18}$$

Figure 3.2 is intended to represent this idea.

Of course, this only works if the interaction details (that is, the operator itself) depend on the density ρ. That this can be made to be the case is the work of the remainder of the thesis.

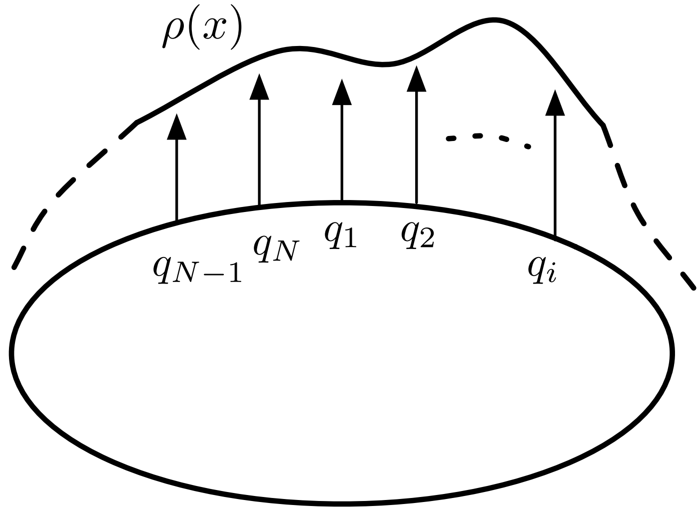

Figure 3.2: The idea behind our fluid limit

Chapter 4

Fluid Approximation

In this chapter I will describe the central novelty in my work: that is the construction of a (dramatically) reduced system of integro-differential equations that describe the evolution of certain marginals of our evolving probability density F. I will begin with a discussion of the important topic of local equilibrium.

From the local equilibrium we will derive a pair of integro-differential equations for what I call the "finite-N fluid" variables. We will see that there is a natural entropy associated to these equations that the dynamics dissipates.

4.1 Local Equilibrium

The best description of local equilibrium from a physics perspective I have found is Spohn's 1991 book [33] and I refer the reader to Part I, Chapter 2 for an excellent discussion. For a more precise perspective consult Kipnis and Landim [27]. In very broad terms the idea is as follows.

One assumes that at a point x the motion of particles is vigorous enough to drive them to a local equilibrium with local conserved quantities (i.e. local momentum, energy). One further assumes that there are so many particles interacting relatively weakly with their distant neighbors that at a different point in the space the particles don't know what is happening at x and so they reach a different equilibrium. This leads to a slowly varying (in space) equilibrium.

To make this more precise we begin with some definitions.

Definition 4.1.1. *Let F be a solution to equation* (2.2.2) *and define*

$$\rho_N(x,t) = \int_{\mathcal{Q}} \int_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i) F \, d\boldsymbol{p} \, d\boldsymbol{q}, \tag{4.1.1}$$

$$\mu_N(x,t) = \int_{\mathcal{Q}} \int_{\mathbb{R}^N} \sum_{i=1}^{N} p_i \delta(x - q_i) F \, d\boldsymbol{p} \, d\boldsymbol{q}. \tag{4.1.2}$$

We will refer to ρ_N and μ_N as finite-N fluid marginals*.*

Remark 4.1.1. Heuristically these functions count respectively the average mass, momentum of particles at a point $x \in \mathbb{T}$. A more "reasonable" definition (following Spohn [33]) would be to define

$$\bar{\rho}_N(B_x,t) = \frac{1}{|B_x|} \int_{\mathcal{Q}} \int_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \chi_{B_x}(q_i) F \, d\boldsymbol{p} \, d\boldsymbol{q}, \tag{4.1.3}$$

$$\bar{\mu}_N(B_x,t) = \frac{1}{|B_x|} \int_{\mathcal{Q}} \int_{\mathbb{R}^N} \sum_{i=1}^{N} p_i \chi_{B_x}(q_i) F \, d\boldsymbol{p} \, d\boldsymbol{q}, \tag{4.1.4}$$

which are precisely the average mass, momentum of particles in the ball B_x centered at x. Formally, taking the limit $|B_x| \to 0$ establishes our definition.

Now, the evolution of the phase space density F (solution to equation (2.2.2)) dissipates the global entropy given in (2.3.2) as it evolves toward $\mathcal{G}_o$ at which point the distribution remains fixed in time. To understand the dynamics of ρ_N and μ_N we need a local equilibrium. We move toward that now.

First note there is an affine subspace L_{ρ_N,μ_N} of densities that have ρ_N, μ_N as marginals:

$$L_{\rho_N,\mu_N} = \Bigg\{ F : \rho_N(x,t) = \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i) F \; d\boldsymbol{p}\, d\boldsymbol{q}, \qquad \mu_N(x,t) = \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} p_i \delta(x - q_i) F \; d\boldsymbol{p}\, d\boldsymbol{q}. \Bigg\}. \tag{4.1.5}$$

Instead of tracking the entire subspace L_{ρ_N,μ_N} we will follow just the element of it that minimizes the entropy. The following lemma demonstrates the existence of such an element. This special density will be the basis for the construction of the "finite-N" fluid equations to follow.

Lemma 4.1.1. *Recall equation* (2.3.2) *which we repeat here:*

$$\mathcal{H}[F; \mathcal{G}_o] = \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} F \log\left(\frac{F}{\mathcal{G}_o}\right) - F + \mathcal{G}_o \; d\boldsymbol{p}\, d\boldsymbol{q}\,. \tag{4.1.6}$$

The minimum of this entropy on the set L_{ρ_N,μ_N} is achieved by

$$\mathcal{G}[\rho_N, \mu_N] = \frac{1}{\sqrt{\det(2\pi\theta \boldsymbol{M})}} \exp\Bigg(-\frac{1}{\theta}\Bigg(\sum_{i=1}^{N} \frac{m_i}{2} \left(\frac{p_i}{m_i} - \frac{\mu_N(q_i,t)}{\rho_N(q_i,t)}\right)^2 - \sum_{i=1}^{N} m_i \frac{\delta S^*}{\delta \rho_N}[\rho_N](q_i,t) + \Phi(\boldsymbol{q}) + S\left[\frac{\delta S^*}{\delta \rho_N}[\rho_N]\right] \Bigg)\Bigg), \tag{4.1.7}$$

where $S^*[\rho_N]$ is the Legendre dual to

$$S[\eta] = \theta \log \int\limits_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q}\,. \tag{4.1.8}$$

We will refer to $\mathcal{G}$ as the local equilibrium, *or* modulated Gibbs distribution *for our system.*

Proof. Let F be a solution to equation (2.2.2) and consider the fluid marginals of F

$$\rho_N(x,t) = \int_{\mathcal{Q}}\int_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i)\, F \; d\boldsymbol{p}\, d\boldsymbol{q}\,, \tag{4.1.9}$$

$$\mu_N(x,t) = \int_{\mathcal{Q}}\int_{\mathbb{R}^N} \sum_{i=1}^{N} p_i \delta(x - q_i)\, F \; d\boldsymbol{p}\, d\boldsymbol{q}\,. \tag{4.1.10}$$

To simplify notation somewhat from now on I will completely suppress the t dependence. We want to minimize $\mathcal{H}[F;\mathcal{G}_o]$ over the set of solutions to the forward Kolmogorov equation (2.2.2) that have ρ_N and μ_N as fluid marginals. We also insist that $\int_{\mathcal{Q}}\int_{\mathbb{R}^N} F\, d\boldsymbol{p}\, d\boldsymbol{q} = 1$. Taking all these constraints into account means we must extremize the functional

$$\begin{aligned} L[F,\lambda_0,\lambda_1,\lambda_2] = \int_{\mathcal{Q}}\int_{\mathbb{R}^N} F\log\left(\frac{F}{\mathcal{G}_o}\right) - F + \mathcal{G}_o \; d\boldsymbol{p}\, d\boldsymbol{q} + \frac{\lambda_0}{\theta}\left(1 - \int_{\mathcal{Q}}\int_{\mathbb{R}^N} F\, d\boldsymbol{p}\, d\boldsymbol{q}\right) \\ + \int_0^1 \frac{\lambda_1(x)}{\theta}\left(\rho_N(x) - \int_{\mathcal{Q}}\int_{\mathbb{R}^N} \sum_{i=1}^{N} m_i\delta(x - q_i)\, F\, d\boldsymbol{p}\, d\boldsymbol{q}\right) dx \\ + \int_0^1 \frac{\lambda_2(x)}{\theta}\left(\mu_N(x) - \int_{\mathcal{Q}}\int_{\mathbb{R}^N} \sum_{i=1}^{N} p_i\delta(x - q_i) F\, d\boldsymbol{p}\, d\boldsymbol{q}\right) dx\,. \end{aligned} \tag{4.1.11}$$

The innocuous θ will have its presence justified shortly. It is straightforward to check that

$$\frac{\delta L}{\delta F} = \log\left(\frac{F}{\mathcal{G}_o}\right) - \frac{\lambda_0}{\theta} - \frac{1}{\theta}\sum_{i=1}^{N} m_i\lambda_1(q_i) - \frac{1}{\theta}\sum_{i=1}^{N} p_i\lambda_2(q_i)\,, \tag{4.1.12}$$

which implies that

$$F_{\text{ext}} = \mathcal{G}_o \exp\left(\frac{1}{\theta}\left(\lambda_0 + \sum_{i=1}^{N} m_i\lambda_1(q_i) + \sum_{i=1}^{N} p_i\lambda_2(q_i)\right)\right) \tag{4.1.13}$$

$$= \frac{1}{\sqrt{\det(2\pi\theta\boldsymbol{M})}Z_o}\exp\left(\frac{1}{\theta}\left(\lambda_0 + \sum_{i=1}^{N} m_i\lambda_1(q_i)\right.\right. \tag{4.1.14}$$

$$\left.\left. + \sum_{i=1}^{N} p_i\lambda_2(q_i) - \sum_{i=1}^{N}\frac{p_i^2}{2m_i} - \Phi(\boldsymbol{q})\right)\right)\,. \tag{4.1.15}$$

A Useful Identity

$$\sum_{i=1}^{N} p_i\lambda_2(q_i) - \sum_{i=1}^{N}\frac{p_i^2}{2m_i} = -\sum_{i=1}^{N}\left[\frac{1}{2m_i}\left(p_i - m_i\lambda_2(q_i)\right)^2 - \frac{m_i}{2}\lambda_2^2(q_i)\right] . \tag{4.1.16}$$

Now we enforce the conditions to find the λs.

Condition 1

$$\int_{\mathcal{Q}}\int_{\mathbb{R}^N} F_{\text{ext}}\, d\boldsymbol{p}\, d\boldsymbol{q} = 1\,, \tag{4.1.17}$$

which implies we must have

$$\frac{1}{Z_o}\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\left(\sum_{i=1}^{N} m_i\left(\frac{1}{2}\lambda_2^2(q_i) + \lambda_1(q_i)\right) - \Phi(\boldsymbol{q})\right)\right)$$
$$\underbrace{\frac{1}{\sqrt{\det\left(2\pi\theta\boldsymbol{M}\right)}}\int_{\mathbb{R}^N} \exp\left(-\frac{1}{\theta}\sum_{i=1}^{N}\frac{1}{2m_i}\left(p_i - m_i\lambda_2(q_i)\right)^2\right) d\boldsymbol{p}}_{=1}\, d\boldsymbol{q} = \exp\left(-\frac{1}{\theta}\lambda_0\right) . \tag{4.1.18}$$

Hence, we find

$$\begin{aligned}\lambda_0 &= -\theta\log\left[\frac{1}{Z_o}\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\left(\sum_{i=1}^{N} m_i\left(\frac{1}{2}\lambda_2^2(q_i) + \lambda_1(q_i)\right) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q}\right] \\ &= \theta\log Z_o - \theta\log\left[\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\left(\sum_{i=1}^{N} m_i\left(\frac{1}{2}\lambda_2^2(q_i) + \lambda_1(q_i)\right) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q}\right] .\end{aligned} \tag{4.1.19}$$

To ease notation make the definitions

$$\eta(q_i) = \frac{1}{2}\lambda_2^2(q_i) + \lambda_1(q_i)\,, \tag{4.1.20}$$

$$S\left[\eta\right] = \theta\log\left[\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\left(\sum_{i=1}^{N} m_i\eta(q_i) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q}\right] , \tag{4.1.21}$$

to get

$$\lambda_0 = \theta\log Z_o - S\left[\eta\right] . \tag{4.1.22}$$

Conditions 2 and 3

We require

$$\int_0^1 \rho_N(x)\delta\lambda_1(x)\,dx = \int\limits_{\mathcal{Q}}\int\limits_{\mathbb{R}^N}\sum_{i=1}^{N} m_i\delta\lambda_1(q_i)F_{\text{ext}}\,d\boldsymbol{p}\,d\boldsymbol{q}\ \forall \text{ admissible } \delta\lambda_1\,, \tag{4.1.23}$$

$$\int_0^1 \mu_N(x)\delta\lambda_2(x)\,dx = \int\limits_{\mathcal{Q}}\int\limits_{\mathbb{R}^N}\sum_{i=1}^{N} p_i\delta\lambda_2(q_i)F_{\text{ext}}\,d\boldsymbol{p}\,d\boldsymbol{q}\ \forall \text{ admissible } \delta\lambda_2\,, \tag{4.1.24}$$

where by "admissible" we mean that the deviations $\delta\lambda_i$ must be smooth and consistent with the boundary conditions—that is, we require $\delta\lambda_i \in C^\infty$ and periodic.

We start with equation (4.1.23) using what we know about λ_o to find (the $\boldsymbol{p}$ integral leaves the equation in the same way as above and the Z_o is canceled by it's appearance in λ_0)

$$\begin{aligned}\int_0^1 &\rho_N(x)\delta\lambda_1(x)\,dx \\ &= \int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i\delta\lambda_1(q_i)\exp\left(\frac{1}{\theta}\left(\sum_{i=1}^{N} m_i\eta(q_i) - \Phi(\boldsymbol{q}) - S\left[\eta\right]\right)\right)\,d\boldsymbol{q}\,.\end{aligned} \tag{4.1.25}$$

Equation (4.1.24) is slightly more complicated:

$$\int_0^1 \mu_N(x)\delta\lambda_2(x)\,dx = \int\limits_{\mathcal{Q}} \mathcal{I}(\boldsymbol{q})\exp\left(\frac{1}{\theta}\left(\sum_{i=1}^{N} m_i\eta(q_i) - \Phi(\boldsymbol{q}) - S\left[\eta\right]\right)\right)\,d\boldsymbol{q}\,, \tag{4.1.26}$$

where

$$\mathcal{I}(\boldsymbol{q}) = \frac{1}{\sqrt{\det\left(2\pi\theta\boldsymbol{M}\right)}}\int\limits_{\mathbb{R}^N}\sum_{i=1}^{N} p_i\delta\lambda_2(q_i)\exp\left(-\frac{1}{\theta}\sum_{i=1}^{N}\frac{1}{2m_i}\left(p_i - m_i\lambda_2(q_i)\right)^2\right)\,d\boldsymbol{p}\,. \tag{4.1.27}$$

Expanding $p_i = (p_i - m_i\lambda_2(q_i)) + m_i\lambda_2(q_i)$ we see

$$\mathcal{I}(\boldsymbol{q}) = \sum_{i=1}^{N} m_i\lambda_2(q_i)\delta\lambda_2(q_i)\,, \tag{4.1.28}$$

and so the μ_N condition becomes

$$
\begin{aligned}
&\int_0^1 \mu_N(x)\delta\lambda_2(x)\,dx \\
&= \int_{\mathcal{Q}} \sum_{i=1}^{N} m_i\lambda_2(q_i)\delta\lambda_2(q_i)\exp\left(\frac{1}{\theta}\left(\sum_{i=1}^{N} m_i\eta(q_i) - \Phi(\boldsymbol{q}) - S\left[\eta\right]\right)\right) d\boldsymbol{q}\,. \quad (4.1.29)
\end{aligned}
$$

Comparing equation (4.1.29) and equation (4.1.25) and picking $\delta\lambda_1 = \lambda_2\delta\lambda_2$ we see

$$
\int_0^1 \rho_N(x)\lambda_2(x)\delta\lambda_2(x)\,dx = \int_0^1 \mu_N(x)\delta\lambda_2(x)\,dx \qquad \forall\ \delta\lambda_2\,, \tag{4.1.30}
$$

which means we must choose

$$
\lambda_2(x) = \frac{\mu_N(x)}{\rho_N(x)} := u_N(x)\,. \tag{4.1.31}
$$

Also note that by substituting Definition (4.1.21) into equation (4.1.25) we see

$$
\int_0^1 \rho_N(x)\delta\lambda_1(x)\,dx = \frac{\int_{\mathcal{Q}} \sum_{i=1}^{N} m_i\delta\lambda_1(q_i)\exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j\eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q}}{\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j\eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q}} \tag{4.1.32}
$$

$$
= \int_0^1 \frac{\delta S}{\delta\eta}(x)\delta\lambda_1(x)\,dx\,, \tag{4.1.33}
$$

hence $\rho_N = \frac{\delta S}{\delta\eta}\left[\eta\right]$. From work in Section A.3 we know that S is a convex functional and so there exists a convex Legendre dual S^* so that $\eta = \frac{\delta S^*}{\delta\rho_N}\left[\rho_N\right]$.

These considerations combine to show that the minimum entropy solution to equation (2.2.2) subject to the fluid marginals constraint (4.1.1) is given as a functional

$$
\begin{aligned}
F_{\text{ext}} &= \mathcal{G}\left[\rho_N, \mu_N\right] \\
&= \frac{1}{\sqrt{\det\left(2\pi\theta \boldsymbol{M}\right)}} \exp\Bigg(-\frac{1}{\theta}\Bigg(\sum_{i=1}^{N} \frac{m_i}{2}\left(\frac{p_i}{m_i} - \frac{\mu_N(q_i)}{\rho_N(q_i)}\right)^2 \\
&\qquad - \sum_{i=1}^{N} m_i \frac{\delta S^*}{\delta \rho_N}\left[\rho_N\right](q_i) + \mathit{\Phi}(\boldsymbol{q}) + S\left[\frac{\delta S^*}{\delta \rho_N}\left[\rho_N\right]\right]\Bigg)\Bigg). \qquad (4.1.34)
\end{aligned}
$$

□

Remark 4.1.2. It will prove convenient in the following material to note that we can view $\mathcal{G}$ as a functional of an alternate pair of variables ρ_N and $u_N = \mu_N/\rho_N$ and to write $\frac{\delta S^*}{\delta \rho_N}[\rho_N] = \eta_N$.

4.2 "Finite-N" Fluid Equations

Here is the big idea: The full unscaled system dissipates the entropy

$$
\mathcal{H}\left[F; \mathcal{G}_o\right] = \int_{\mathcal{Q}} \int_{\mathbb{R}^N} F \log\left(\frac{F}{\mathcal{G}_o}\right) - F + \mathcal{G}_o \, d\boldsymbol{p} \, d\boldsymbol{q}\,, \qquad (4.2.1)
$$

and if we are given functions ρ_N, μ_N then minimizing $\mathcal{H}$ over those F that have ρ_N, μ_N as marginals gives $\mathcal{G}$. Now, if $F = \mathcal{G}$ solves the forward Kolmogorov equation we have a closed system for ρ_N, μ_N and the dynamics of ρ_N, μ_N dissipates the entropy $\mathcal{H}\left[\mathcal{G}; \mathcal{G}_o\right]$.

We make this more precise with the following two lemmas.

Lemma 4.2.1. *In order for the modulated Gibbs distribution $\mathcal{G}\left[\rho_N, \mu_N\right]$ to solve the forward Kolmogorov equation* (2.2.2) *we must have*

$$
\partial_t \rho_N + \partial_x \mu_N = 0\,, \qquad (4.2.2)
$$

$$
\partial_t \mu_N + \partial_x\left(u_N^2 \rho_N\right) + \rho_N \partial_x \eta_N = V\left[\mu_N/\rho_N\right]\,, \qquad (4.2.3)
$$

where

$$V[u] = -\int\limits_{\mathcal{Q}} \frac{1}{Z} \sum_{i=1}^{N} \delta\left(x - q_i\right) \left[\boldsymbol{\Xi} \boldsymbol{u}\right]_i \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta\left(q_j\right) - \Phi\left(\boldsymbol{q}\right)\right)\right) d\boldsymbol{q}\,, \tag{4.2.4}$$

with $\boldsymbol{u} = (u(q_1), u(q_2), \ldots, u(q_N))$.

Lemma 4.2.2. *The evolution of equations* (4.2.2) *and* (4.2.3) *dissipate the entropy*

$$\mathcal{H}\left[\mathcal{G}; \mathcal{G}_o\right] = \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \mathcal{G} \log\left(\frac{\mathcal{G}}{\mathcal{G}_o}\right) \, d\boldsymbol{p}\, d\boldsymbol{q}\,. \tag{4.2.5}$$

Proof of Lemma 4.2.1. We begin by rewriting equation (2.2.2) here for reference

$$\partial_t F + \boldsymbol{M}^{-1}\boldsymbol{p} \cdot \nabla_{\boldsymbol{q}} F - \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} F = \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\left(\theta \nabla_{\boldsymbol{p}} F + \boldsymbol{M}^{-1}\boldsymbol{p} F\right)\right]. \tag{4.2.6}$$

Now, note that equation (4.2.2) is relatively straightforward

$$\partial_t \rho_N = \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i) \partial_t F \, d\boldsymbol{p}\, d\boldsymbol{q} \tag{4.2.7}$$

$$= -\int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i) \nabla_{\boldsymbol{q}} \cdot \left(\boldsymbol{M}^{-1}\boldsymbol{p} F\right) \, d\boldsymbol{p}\, d\boldsymbol{q} \tag{4.2.8}$$

$$+ \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i) \nabla_{\boldsymbol{p}} \cdot \left(\nabla_{\boldsymbol{q}} \Phi F\right) \, d\boldsymbol{p}\, d\boldsymbol{q} \tag{4.2.9}$$

$$+ \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i) \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi}\left(\theta \nabla_{\boldsymbol{p}} F + \boldsymbol{M}^{-1}\boldsymbol{p} F\right)\right] \, d\boldsymbol{p}\, d\boldsymbol{q}\,. \tag{4.2.10}$$

The last two terms in the right-hand side are zero by the Divergence theorem applied to the $\boldsymbol{p}$ integral. We are left with

$$\partial_t \rho_N = -\int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i) \nabla_{\boldsymbol{q}} \cdot \left(\boldsymbol{M}^{-1}\boldsymbol{p} F\right) \, d\boldsymbol{p}\, d\boldsymbol{q}\,. \tag{4.2.11}$$

Proceeding formally we note that

$$- \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \delta(x - q_i) \nabla_{\boldsymbol{q}} \cdot \left(\boldsymbol{M}^{-1} \boldsymbol{p} F \right) \, d\boldsymbol{p} \, d\boldsymbol{q}$$

$$= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} m_i \nabla_{\boldsymbol{q}} \delta(x - q_i) \cdot \boldsymbol{M}^{-1} \boldsymbol{p} F \, d\boldsymbol{p} \, d\boldsymbol{q} \,, \quad (4.2.12)$$

but the elements of the $\nabla_{\boldsymbol{q}} \delta(x - q_i)$ factor are all zero except for the i^{th} and that one is $-\partial_x \delta(x - q_i)$ and so we have

$$\partial_t \rho_N = - \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} p_i \partial_x \delta(x - q_i) F \, d\boldsymbol{p} \, d\boldsymbol{q} \quad (4.2.13)$$

$$= -\partial_x \mu_N \,. \quad (4.2.14)$$

Note that this part of the proof did not make use of the Gibbs distribution. That is because this part of the fluid equations is always true. The momentum flow is where we must use the Gibbs solution to equation (4.2.6). We now move on to the more complicated equation (4.2.3). Using equation (4.2.6) and suppressing the N dependence for the moment we see

$$\partial_t \mu + \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} p_i \delta\left(x - q_i\right) \boldsymbol{M}^{-1} p \cdot \nabla_{\boldsymbol{q}} F \; d\boldsymbol{p} \, d\boldsymbol{q}$$

$$- \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} p_i \delta\left(x - q_i\right) \nabla_{\boldsymbol{q}} \Phi \cdot \nabla_{\boldsymbol{p}} F \, d\boldsymbol{p} \, d\boldsymbol{q}$$

$$= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} p_i \delta\left(x - q_i\right) \nabla_{\boldsymbol{p}} \cdot \left[\boldsymbol{\Xi} \left(\theta \nabla_{\boldsymbol{p}} F + \boldsymbol{M}^{-1} \boldsymbol{p} \right) F \right] \; d\boldsymbol{p} \, d\boldsymbol{q} \,. \quad (4.2.15)$$

It is straightforward to verify that

$$\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N} p_i\delta\left(x-q_i\right)\boldsymbol{M}^{-1}p\cdot\nabla_{\boldsymbol{q}}F\;d\boldsymbol{p}\,d\boldsymbol{q}=\partial_x\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N}\frac{p_i^2}{m_i}\delta\left(x-q_i\right)F\,d\boldsymbol{p}\,d\boldsymbol{q}\,, \tag{4.2.16}$$

$$-\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N} p_i\delta\left(x-q_i\right)\nabla_{\boldsymbol{q}}\varPhi\cdot\nabla_{\boldsymbol{p}}F\,d\boldsymbol{p}\,d\boldsymbol{q}=\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N}\delta\left(x-q_i\right)\partial_{q_i}\varPhi F\,d\boldsymbol{p}\,d\boldsymbol{q}\,, \tag{4.2.17}$$

$$\begin{aligned}\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N} p_i\delta\left(x-q_i\right)\nabla_{\boldsymbol{p}}\cdot\left[\boldsymbol{\varXi}\left(\theta\nabla_{\boldsymbol{p}}F+\boldsymbol{M}^{-1}\boldsymbol{p}F\right)\right]\;d\boldsymbol{p}\,d\boldsymbol{q}&\\ =-\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N}\delta\left(x-q_i\right)\left[\boldsymbol{\varXi}\left(\theta\nabla_{\boldsymbol{p}}F+\boldsymbol{M}^{-1}\boldsymbol{p}F\right)\right]_i\;d\boldsymbol{p}\,d\boldsymbol{q}\,.&\end{aligned} \tag{4.2.18}$$

Hence, we can transform equation (4.2.15) into

$$\begin{aligned}\partial_t\mu+\partial_x\underbrace{\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N}\frac{p_i^2}{m_i}\delta\left(x-q_i\right)F\,d\boldsymbol{p}\,d\boldsymbol{q}}_{A}&\\ +\underbrace{\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N}\delta\left(x-q_i\right)\partial_{q_i}\varPhi F\,d\boldsymbol{p}\,d\boldsymbol{q}}_{B}&\\ =\underbrace{-\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N}\delta\left(x-q_i\right)\left[\boldsymbol{\varXi}\left(\theta\nabla_{\boldsymbol{p}}F+\boldsymbol{M}^{-1}\boldsymbol{p}\right)F\right]_i\;d\boldsymbol{p}\,d\boldsymbol{q}}_{C}\;.&\end{aligned} \tag{4.2.19}$$

Now, for $F=\mathcal{G}$ it is possible to calculate A,B, and C.

$$\begin{aligned}A&=\int_{\mathcal{Q}}\int_{\mathbb{R}^N}\sum_{i=1}^{N}\frac{p_i^2}{m_i}\delta\left(x-q_i\right)\mathcal{G}\,d\boldsymbol{p}\,d\boldsymbol{q}\\ &=\frac{1}{Z}\int_{\mathcal{Q}}\sum_{i=1}^{N}\delta\left(x-q_i\right)I_i\left(\boldsymbol{q}\right)\exp\left(\frac{1}{\theta}\left(\sum_{j=-1}^{N}m_j\eta\left(q_j\right)-\varPhi\left(\boldsymbol{q}\right)\right)\right)d\boldsymbol{q}\,,\end{aligned} \tag{4.2.20}$$

where

$$I_i(\boldsymbol{q}) = \frac{1}{\sqrt{\det(2\pi \boldsymbol{M}\theta)}} \int\limits_{\mathbb{R}^N} \frac{p_i^2}{m_i} \exp\left(-\frac{1}{\theta}\left(\sum_{j=1}^{N} \frac{1}{2m_j}\left(p_j - m_j u(q_j)\right)^2\right)\right) d\boldsymbol{p}\,. \tag{4.2.21}$$

Using the fact that $p_i^2 = (p_i - m_i u(q_i))^2 + 2m_i u(q_i)(p_i - m_i u(q_i)) + m_i^2 u(q_i)$ and Lemma A.2.1 we have that

$$I_i(\boldsymbol{q}) = \theta + m_i (u(q_i))^2\ , \tag{4.2.22}$$

which means that

$$\begin{aligned} A &= \theta \int\limits_{\mathcal{Q}} \frac{1}{Z} \sum_{i=1}^{N} \delta(x - q_i) \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q} \\ &\quad + \int\limits_{\mathcal{Q}} \frac{1}{Z} \sum_{i=1}^{N} m_i (u(q_i))^2 \delta(x - q_i) \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q} \\ &= \boxed{\theta \int\limits_{\mathcal{Q}} \frac{1}{Z} \sum_{i=1}^{N} \delta(x - q_i) \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q}} + u^2 \rho\,. \end{aligned} \tag{4.2.23}$$

Now

$$\begin{aligned} B &= \int\limits_{\mathcal{Q}} \int\limits_{\mathbb{R}^N} \sum_{i=1}^{N} \delta(x - q_i)\, \partial_{q_i} \Phi(\boldsymbol{q})\, \mathcal{G}\, d\boldsymbol{p}\, d\boldsymbol{q} \\ &= \frac{1}{Z} \int\limits_{\mathcal{Q}} \sum_{i=1}^{N} \delta(x - q_i)\, \partial_{q_i} \Phi(\boldsymbol{q}) \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q} \\ &= \frac{1}{Z} \int\limits_{\mathcal{Q}} \sum_{i=1}^{N} m_i \delta(x - q_i)\, \partial_x \eta(q_i) \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q} \\ &\quad - \frac{\theta}{Z} \int\limits_{\mathcal{Q}} \sum_{i=1}^{N} \delta(x - q_i)\, \partial_{q_i} \left[\exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right)\right] d\boldsymbol{q} \\ &= \rho \partial_x \eta - \partial_x \boxed{\theta \int\limits_{\mathcal{Q}} \frac{1}{Z} \sum_{i=1}^{N} \delta(x - q_i) \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right) d\boldsymbol{q}}\,. \end{aligned} \tag{4.2.24}$$

The cancellation in the boxed terms will prove *very* convenient. Finally, we write

$$
\begin{aligned}
C &= -\int_{\mathcal{Q}} \int_{\mathbb{R}^N} \sum_{i=1}^{N} \delta\left(x - q_i\right) \left[\boldsymbol{\Xi}\left(\theta \nabla_{\boldsymbol{p}} \mathcal{G} + \boldsymbol{M}^{-1}\boldsymbol{p}\right)\mathcal{G}\right]_i \, d\boldsymbol{p}\, d\boldsymbol{q} \\
&= -\int_{\mathcal{Q}} \int_{\mathbb{R}^N} \sum_{i=1}^{N} \delta\left(x - q_i\right) \left[\boldsymbol{\Xi}\left(\theta\left(\frac{\boldsymbol{u} - \cancel{\boldsymbol{M}^{-1}\boldsymbol{p}}}{\theta}\right)\mathcal{G} + \cancel{\boldsymbol{M}^{-1}\boldsymbol{p}\mathcal{G}}\right)\right] \, d\boldsymbol{p}\, d\boldsymbol{q} \\
&= -\int_{\mathcal{Q}} \frac{1}{Z} \sum_{i=1}^{N} \delta\left(x - q_i\right) \left[\boldsymbol{\Xi}\boldsymbol{u}\right]_i \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta\left(q_j\right) - \Phi\left(\boldsymbol{q}\right)\right)\right) d\boldsymbol{q} \,. \qquad (4.2.25)
\end{aligned}
$$

With these expressions in hand we can say that if $\mathcal{G}$ is to be a solution we must require that ρ and μ satisfy the following equations

$$
\partial_t \rho_N + \partial_x \mu_N = 0 \,, \qquad (4.2.26)
$$

$$
\begin{aligned}
&\partial_t \mu_N + \partial_x \left(u_N^2 \rho_N\right) + \rho_N \partial_x \eta_N = \\
&\qquad -\int_{\mathcal{Q}} \frac{1}{Z} \sum_{i=1}^{N} \delta\left(x - q_i\right) \left[\boldsymbol{\Xi}\boldsymbol{u}\right]_i \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta\left(q_j\right) - \Phi\left(\boldsymbol{q}\right)\right)\right) d\boldsymbol{q} \,. \qquad (4.2.27)
\end{aligned}
$$

$\square$

We now move on to the Entropy dissipation.

Proof of Lemma 4.2.2. We begin with

$$
\mathcal{H}\left[\mathcal{G}; \mathcal{G}_o\right] = \int_{\mathcal{Q}} \int_{\mathbb{R}^N} \mathcal{G} \log\left(\frac{\mathcal{G}}{\mathcal{G}_o}\right) \, d\boldsymbol{p}\, d\boldsymbol{q} \,. \qquad (4.2.28)
$$

Expanding this directly we have

$$
\begin{aligned}
\mathcal{H}\left[\mathcal{G}; \mathcal{G}_o\right] &= \frac{1}{\theta Z\left[\eta\right]} \int_{\mathcal{Q}} \sum_{j=1}^{N} m_j \eta\left(q_j\right) \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta\left(q_j\right) - \Phi\left(\boldsymbol{q}\right)\right)\right) d\boldsymbol{q} \\
&\quad + \frac{1}{\theta Z\left[\eta\right]} \int_{\mathcal{Q}} \sum_{j=1}^{N} \frac{m_j \left(u\left(q_j\right)\right)^2}{2} \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta\left(q_j\right) - \Phi\left(\boldsymbol{q}\right)\right)\right) d\boldsymbol{q} \\
&\quad + \log\left(\int_{\mathcal{Q}} \exp\left(-\frac{1}{\theta}\Phi\left(\boldsymbol{q}\right)\right) d\boldsymbol{q}\right) - \log Z\left[\eta\right] . \qquad (4.2.29)
\end{aligned}
$$

For the rest of the derivation let us make a simplification in the notation. Define

$$\mathcal{G}_\eta\left(\boldsymbol{q}\right) = \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta\left(q_j\right) - \Phi\left(\boldsymbol{q}\right)\right)\right). \tag{4.2.30}$$

It is straightforward to find the variation in $\mathcal{H}\left[\mathcal{G};\mathcal{G}_o\right]$:

$$\begin{aligned}
\delta\mathcal{H} = &\cancel{\frac{1}{\theta Z}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i \delta\eta\left(q_i\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q}} \\
&+ \frac{1}{\theta^2 Z}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i \eta\left(q_i\right)\sum_{j=1}^{N} m_j \delta\eta\left(q_j\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q} \\
&- \frac{1}{\theta^2 Z^2}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i \eta\left(q_i\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q}\int\limits_{\mathcal{Q}}\sum_{j=1}^{N} m_j \delta\eta\left(q_j\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q} \\
&+ \frac{1}{\theta^2 Z}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} \frac{m_i\left(u\left(q_i\right)\right)^2}{2}\sum_{j=1}^{N} m_j \delta\eta\left(q_j\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q} \\
&- \frac{1}{\theta^2 Z^2}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} \frac{m_i\left(u\left(q_i\right)\right)^2}{2}\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q}\int\limits_{\mathcal{Q}}\sum_{j=1}^{N} m_j \delta\eta\left(q_j\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q} \\
&\cancel{-\frac{1}{\theta Z}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i \delta\eta\left(q_i\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q}} \\
&+ \frac{1}{\theta Z}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i u\left(q_i\right)\delta u\left(q_i\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q}\,.
\end{aligned} \tag{4.2.31}$$

From this calculation we find

$$\begin{aligned}
\frac{\delta\mathcal{H}}{\delta\eta}\left(x\right) &= \frac{1}{\theta^2 Z}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i\left(\eta_i + \frac{u_i^2}{2}\right)\sum_{j=1}^{N} m_j \delta\left(x - q_j\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q} \\
&\quad - \frac{1}{\theta^2 Z^2}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i\left(\eta_i + \frac{u_i^2}{2}\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i \delta\left(x - q_i\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q} \\
&= \int_0^1 \frac{1}{\theta}\frac{\delta^2 S}{\delta\eta^2}\left(x,z\right)\left(\eta\left(z\right) + \frac{\left(u\left(z\right)\right)^2}{2}\right)\, dz
\end{aligned} \tag{4.2.32}$$

$$\frac{\delta\mathcal{H}}{\delta u}\left(x\right) = \frac{1}{\theta Z}\int\limits_{\mathcal{Q}}\sum_{i=1}^{N} m_i u\left(q_i\right)\delta\left(x - q_i\right)\mathcal{G}_\eta\left(\boldsymbol{q}\right)\, d\boldsymbol{q} = \frac{1}{\theta}u(x)\rho(x)\,. \tag{4.2.33}$$

We also have

$$\frac{\delta u}{\delta \rho}(x,y) = -\frac{\mu(x)}{\rho^2(x)}\delta\left(x-y\right) = -\frac{u(x)}{\rho(x)}\delta(x-y)\,, \tag{4.2.34}$$

$$\frac{\delta u}{\delta \mu}(x,y) = \frac{1}{\rho(x)}\delta(x-y)\,, \tag{4.2.35}$$

$$\frac{\delta \eta}{\delta \rho}(x,y) = \frac{\delta^2 S^*}{\delta \rho^2}(x,y)\,. \tag{4.2.36}$$

Now we can write

$$\begin{aligned}
\frac{d}{dt}\mathcal{H}\left[\mathcal{G};\mathcal{G}_o\right] = \int_0^1\int_0^1 & \left[\frac{\delta\mathcal{H}}{\delta u}(x)\frac{\delta u}{\delta\rho}(x,y) + \frac{\delta\mathcal{H}}{\delta\eta}(x)\frac{\delta\eta}{\delta\rho}(x,y)\right]\partial_t\rho(y)\,dxdy \\
& + \int_0^1\int_0^1 \frac{\delta\mathcal{H}}{\delta u}(x)\frac{\delta u}{\delta\mu}(x,y)\partial_t\mu(y)\,dxdy \\
= & -\frac{1}{\theta}\int_0^1 u^2(x)\partial_t\rho(x)\,dx \\
& + \frac{1}{\theta}\int_0^1\int_0^1 \frac{\delta^2 S^*}{\delta\rho^2}(x,y)\int_0^1\frac{\delta^2 S}{\delta\eta^2}(x,z)\left(\eta(z)+\frac{u^2(z)}{2}\right)\,dz\,\partial_t\rho(y)\,dxdz \\
& \qquad + \frac{1}{\theta}\int_0^1 u(x)\partial_t\mu(x)\,dx \\
= & \frac{1}{\theta}\int_0^1\left(\eta-\frac{u^2}{2}\right)\partial_t\rho + u\partial_t\mu\,dx\,,
\end{aligned} \tag{4.2.37}$$

where we have used the fact that the operators $\frac{\delta^2 S}{\delta\eta^2}$ and $\frac{\delta^2 S^*}{\delta\rho^2}$ are inverses. Now using equations (4.2.2) and (4.2.3) we have (please forgive the mixing of the μ,ρ and u,ρ variable choice)

$$\begin{aligned}
\frac{d}{dt}\mathcal{H}\left[\mathcal{G};\mathcal{G}_o\right] = & \frac{1}{\theta}\int_0^1 u(x)\left(V\left[u\right]-\partial_x\left(u^2\rho\right)-\rho\partial_x\eta\right)\,dx \\
& \qquad - \frac{1}{\theta}\int_0^1\left(\eta(x)-\frac{u^2(x)}{2}\right)\partial_x\mu\,dx \\
= & \frac{1}{\theta}\int_0^1 uV\left[u\right]\,dx + \frac{1}{\theta}\int_0^1\frac{u^2}{2}\partial_x(\rho u)\,dx - \frac{1}{\theta}\int_0^1 u\partial_x\left(u^2\rho\right)\,dx \\
& \qquad - \frac{1}{\theta}\int_0^1\eta\partial_x\left(\rho u\right)\,dx - \frac{1}{\theta}\int_0^1\rho u\partial_x\eta\,dx\,.
\end{aligned} \tag{4.2.38}$$

Now, integration by parts (twice) shows

$$\int_0^1\frac{u^2}{2}\partial_x(\rho u)\,dx = \int_0^1 u\partial_x\left(u^2\rho\right)\,dx\,, \tag{4.2.39}$$

and another shows

$$\int_0^1 \eta\partial_x(\rho u)\,dx = -\int_0^1 \rho u\partial_x\eta\,dx\,. \tag{4.2.40}$$

Hence, we are left with

$$\frac{d}{dt}\mathcal{H}\left[\mathcal{G};\mathcal{G}_o\right] = \frac{1}{\theta}\int_0^1 uV\left[u\right]\,dx \tag{4.2.41}$$

$$= -\frac{1}{\theta}\int_0^1 u(x)\int\limits_{\mathcal{Q}} \frac{1}{Z}\sum_{i=1}^N \delta\left(x-q_i\right)\left[\boldsymbol{\Xi u}\right]_i \mathcal{G}_\eta(\boldsymbol{q})\,d\boldsymbol{q}\,dx \tag{4.2.42}$$

$$= -\int\limits_{\mathcal{Q}} \frac{1}{Z}\sum_{i=1}^N u(q_i)\left[\boldsymbol{\Xi u}\right]_i \mathcal{G}_\eta(\boldsymbol{q})\,d\boldsymbol{q} \tag{4.2.43}$$

$$= -\int\limits_{\mathcal{Q}} \frac{1}{Z}\boldsymbol{u}\cdot\boldsymbol{\Xi u}\,\mathcal{G}_\eta(\boldsymbol{q})\,d\boldsymbol{q} \le 0\,, \tag{4.2.44}$$

using the properties of $\boldsymbol{\Xi}$ in Section A.4. □

Summary

I have formally shown that the full N-particle system can be realized as a coarsening of a pair of partial integro-differential equations. What is more, these “finite-N” equations (or fluid marginals) arise as parameters in a minimizer of relative entropy. The closure is in the spirit of the work done by Eyink and Levermore where they discuss the global dissipation of an entropy. Here I have constructed a local entropy structure and I have not seen such a thing in my reading.

In the next chapter we will see that this structure is formally inherited by the $N \to \infty$ limit.

Chapter 5

Formal Hydrodynamic Limit

In this chapter I will formally investigate some aspects of the $N \to \infty$ limit for the finite-N fluid equations (4.2.2), (4.2.3). The discussion will necessarily be more casual.

We begin by repeating the finite-N fluid equations here:

$$\partial_t \rho_N + \partial_x \mu_N = 0, \tag{5.0.1}$$

$$\partial_t \mu_N + \partial_x \left(u_N^2 \rho_N\right) + \rho_N \partial_x \eta_N = V\left[\mu_N / \rho_N\right] . \tag{5.0.2}$$

As I see it there are three main issues with taking the $N \to \infty$ limit in these equations.

1. The most important question is the simplest: do the limits $\rho_N \to \rho$ and $\mu_N \to \mu$ exist? Are they unique?
2. Supposing 1 is resolved, what is $\lim_{N\to\infty} \eta_N = \lim_{N\to\infty} \frac{\delta S^*}{\delta \rho_N}$?
3. What is $\lim_{N\to\infty} V[u]$?

In the next section I will discuss question 2.

5.1 Discussion of Formal Limit for η_N

Recall that S^* is the Legendre dual of $S[\eta] = \theta \log Z[\eta]$ where

$$Z[\eta] = \int_{\mathcal{Q}} \exp\left(-\frac{1}{\theta}\left(\Phi(\boldsymbol{q}) - \sum_{i=1}^{N} m_i \eta(q_i)\right)\right) d\boldsymbol{q}\,. \tag{5.1.1}$$

Hence, it is natural to begin by investigating the limit behavior of Z.

A word on the potential energy Φ: in order to take a limit we will have to make precise statements about its form. Mimicking gas dynamics we define

$$\Phi(\boldsymbol{q}) = \frac{\alpha^\gamma}{\gamma} \sum_{i=1}^{N} \left(\frac{m_{i-1/2}}{q_j - q_{j-2}}\right)^{\gamma-1}, \tag{5.1.2}$$

where $m_{i-1/2}$ depends "in some way" on m_i, m_{i-1}. What is the form of mass dependence in the potential energy?

Ultimately we want to view the particle positions as approximations to a fluid density as an impulse train, i.e. in the sense that

$$\sum_{i=1}^{N} m_i \delta(x - q_i) \to \rho(x) \text{ as } N \to \infty\,. \tag{5.1.3}$$

Let's investigate this. As $N \to \infty$, formally

$$\int_{q_{j-1}}^{j} \sum_{i=1}^{N} m_i \delta(x - q_i) \phi(x)\, dx \to \int_{q_{j-1}}^{q_j} \rho(x)\phi(x)\, dx\,, \tag{5.1.4}$$

$$m_{j-1}\phi(q_{j-1}) + m_j \phi(q_j) \sim (q_j - q_{j-1}) \frac{\rho(q_j)\phi(q_j) + \rho(q_{j-1})\phi(q_{j-1})}{2}\,. \tag{5.1.5}$$

The last line is the result of the trapezoidal rule on the integral with ρ. So, for things to make sense for general ϕ (we can choose one supported near each of q_j, q_{j-1}) we need

$$m_{j-1} \sim \frac{\rho(q_{j-1})}{2}(q_j - q_{j-1})\,, \tag{5.1.6}$$

$$m_j \sim \frac{\rho(q_j)}{2}(q_j - q_{j-1})\,, \tag{5.1.7}$$

or

$$\frac{m_j + m_{j-1}}{q_j + q_{j-1}} \sim \frac{\rho(q_j) + \rho(q_{j-1})}{2} \sim \rho\left(\frac{q_j + q_{j-1}}{2}\right) , \tag{5.1.8}$$

for nice ρ. This means that if we are to have $\sum_i m_i \delta(x - q_i) \to \rho(x)$ it is necessary that

$$\frac{m_j + m_{j-1}}{q_j + q_{j-1}} \sim \rho\left(\frac{q_j + q_{j-1}}{2}\right) . \tag{5.1.9}$$

Hence, the appropriate definition for $\varPhi$ is

$$\varPhi(\boldsymbol{q}) = \frac{\alpha^\gamma}{\gamma} \sum_{i=1}^{N} \frac{(m_j + m_{j-1})^\gamma}{(q_j - q_{j-1})^{\gamma-1}} . \tag{5.1.10}$$

The need for the extra mass factor will become apparent.

Now, on to the main idea:

$$Z = \int_{\mathcal{Q}} \exp\left(-\frac{1}{\theta}\mathcal{U}(\boldsymbol{q})\right) d\boldsymbol{q} , \tag{5.1.11}$$

where $\mathcal{U}(\boldsymbol{q}) = \varPhi(\boldsymbol{q}) - \sum_{i=1}^{N} m_j \eta(q_j)$.

Note that $\mathcal{U}$ blows up on the collision set ∂Q since

$$\varPhi(\boldsymbol{q}) \sim \sum_{i=2}^{N} \frac{1}{s_j^{\gamma-1}} , \tag{5.1.12}$$

and has a minimum in the interior on $s_2 = s_3 = \cdots = s_N$. Naively we want to use Laplace's method to estimate the value of this integral, but in order to do so we need to know that the argument of the exponential blows up as $N \to \infty$. Recall the toy model discussion in Section 3.5 where we saw that for $\varPhi \sim \sum_{i=1}^{N} \frac{1}{s_j^p}$ we would have near the minimum $\varPhi \sim \text{Constant} \cdot N^{p+2}$ and so by comparison we will have

$$\begin{aligned} \varPhi(\boldsymbol{q}) &= \frac{\alpha^\gamma}{\gamma} \sum_{i=1}^{N} \frac{(m_j + m_{j-1})^\gamma}{(q_j - q_{j-1})^{\gamma-1}} \\ &\sim \text{Constant} \cdot N^{\gamma+1} \cdot \mathcal{O}((m_j + m_{j-1})^\gamma) \cdot (\text{quadratic form}) , \end{aligned} \tag{5.1.13}$$

but the mass contribution must be $\mathcal{O}(1/N)$ so we see

$$\varPhi \sim \mathcal{O}(N) \cdot (\text{quadratic form}) \,. \tag{5.1.14}$$

Remark 5.1.1. Note that I have not mentioned η yet. This is because we are assuming η is bounded and so will not contribute to the question of blow up in the exponential. This is not to say its influence will not be felt as we will see below.

At any rate we meet the formal criterion to apply Laplace's method and so we will get (if there is justice)

$$Z \sim \text{Constant}(N) \times \exp\left(-\frac{1}{\theta}\mathcal{U}(\boldsymbol{q}^*)\right) \,, \tag{5.1.15}$$

where $\mathcal{U}(\boldsymbol{q}^*) = \min\{\mathcal{U}(\boldsymbol{q}) : \boldsymbol{q} \in \mathcal{Q}\}$. This implies

$$S\,[\eta] = \theta \log Z \sim -\mathcal{U}(\boldsymbol{q}^*) + \text{Constant(N)} \,. \tag{5.1.16}$$

We can ignore the last term as we will be after the variation in S and not its actual value.

Now comes the important claim. Consider the following formal manipulation:

$$\mathcal{U}\,(\boldsymbol{q}) = \frac{\alpha^\gamma}{\gamma}\sum_{i=1}^{N}\frac{(m_j + m_{j-1})^\gamma}{(q_j - q_{j-1})^\gamma}(q_j - q_{j-1}) - \sum_{j=1}^{N}\frac{m_j\eta(q_j)}{q_j - q_{j-1}}(q_j - q_{j-1}) \tag{5.1.17}$$

$$\to \frac{\alpha^\gamma}{\gamma}\int_0^1 \rho^\gamma \, dx - \int_0^1 \rho\eta \, dx \,. \tag{5.1.18}$$

This manipulation is another justification for the form of $\varPhi$. There have been liberties taken with respect to the second integral. The mass factor is not the same and yet it has been treated in the same way. I believe this can be corrected.

The point of this manipulation is to deal with the $\mathcal{U}(\boldsymbol{q}^*)$ in the limiting behavior of S. If I can show

$$\sum_{i=1}^{N} m_i\delta(x - q_i^*) \to \rho^*(x) \,, \tag{5.1.19}$$

where

$$\rho^* = \operatorname{argmin}\left\{\frac{\alpha^\gamma}{\gamma}\int_0^1 \rho^\gamma\,dx - \int_0^1 \rho\eta\,dx : \rho\right\}, \tag{5.1.20}$$

we will be able to find the limit for η. Note that the appearance of η is what gives a nontrivial minimum. If it were not in the expression for $\mathcal{U}$ we would only get the minimum of Φ.

The minimization problem (5.1.20) can be solved with standard calculus of variations arguments to give

$$\alpha^\gamma \left(\rho^*\right)^{\gamma-1} = \eta \implies \rho^* = \frac{\eta^{\gamma^*-1}}{\alpha^{\gamma^*}}, \tag{5.1.21}$$

where $\frac{1}{\gamma} + \frac{1}{\gamma^*} = 1$ and then

$$\frac{\alpha^\gamma}{\gamma}\int_0^1 \left(\rho^*\right)^\gamma\,dx - \int_0^1 \rho^*\eta\,dx = -\frac{\alpha^{-\gamma^*}}{\gamma^*}\int_0^1 \eta^{\gamma^*}\,dx\,. \tag{5.1.22}$$

Hence,

$$S\left[\eta\right] \sim \frac{\alpha^{-\gamma^*}}{\gamma^*}\int_0^1 \eta^{\gamma^*}\,dx\,, \tag{5.1.23}$$

$$S^*\left[\rho\right] \sim \frac{\alpha^\gamma}{\gamma}\int_0^1 \rho^\gamma\,dx\,, \tag{5.1.24}$$

at least for the purposes of taking variations. These formal manipulations show that in the limit $N \to \infty$ we will have

$$\frac{\delta S^*}{\delta \rho_N} \to \alpha^\gamma \rho^{\gamma-1}\,. \tag{5.1.25}$$

5.2 Speculation and Conjecture

The hydrodynamic limit for our finite-N fluid system is of great importance to the program of understanding the model hierarchy. This is because the "feeling" at this point is that the hydrodynamic limit represents the fixed point for the map between hierarchy elements in the following sense. Take a finite-N fluid system and apply the compression operator to it. The original and the compressed version should go to the same hydrodynamic limit.

There are questions about this hydrodynamic limit.

- If it is true that it is a fixed point for the compression map, what is the attracting set? That is, could we expand the class of particle interactions beyond nearest-neighbor? One would expect on physical grounds that repeatedly clumping parcels together and averaging would wash out any interaction beyond nearest-neighbor. Is there a class of particle interactions that all approach this hydrodynamic description on repeated averaging?

- How does the unknown function λ come into play? I have made tentative investigations of it, but still not nailed it down. The intuition is that when we move to corrections of the fluid system we will find solvability conditions that will put strong conditions on λ.

Appendix A

Supporting Material

In this section I will include some results I use in this thesis.

A.1 Required Functional Analysis

The following definitions are all from [31].

Definition A.1.1. *Let T be a densely defined linear operator on a Hilbert Space $\mathbb{H}$. Let* $\mathrm{Dom}\,(T^*)$ *be the set of $\phi \in \mathbb{H}$ for which there is an $\eta \in \mathbb{H}$ with*

$$(T\psi, \phi) = (\psi, \eta) \ \ \forall \ \psi \in \mathrm{Dom}\,(T) \ . \tag{A.1.1}$$

For each such $\phi \in \mathrm{Dom}(T^*)$, we define $T^*\phi = \eta$. T^* is called the adjoint of T. By the Riesz Lemma, $\phi \in \mathrm{Dom}\,(T^*)$ if and only if there exists C such that $|(T\psi, \phi)| \leq C\,||\psi||$ for all $\psi \in \mathrm{Dom}(T)$.

Definition A.1.2. *A densely defined operator T on a Hilbert Space is called symmetric (or Hermitian) if $T \subset T^*$, that is if $\mathrm{Dom}\,(T) \subset \mathrm{Dom}\,(T^*)$ and $T\phi = T^*\phi$ for all $\phi \in \mathrm{Dom}\,(T)$. Equivalently, T is symmetric if and only if*

$$(T\phi, \psi) = (\phi, T^*\psi) \ \ \forall \ \phi, \psi \in \mathrm{Dom}\,(T) \ . \tag{A.1.2}$$

Definition A.1.3. *T is called self-adjoint if $T = T^*$, that is if and only if T is symmetric and* $\mathrm{Dom}\,(T) = \mathrm{Dom}\,(T^*)$.

Theorem A.1.1. *(Von Neumann) Let A be a closed densely defined operator and let*

$$\mathrm{Dom}\,(A^* A) = \{\psi \in \mathrm{Dom}\,(A) \mid A\psi \in \mathrm{Dom}\,(A^*)\}\ . \tag{A.1.3}$$

Define $A^* A$ on $\mathrm{Dom}\,(A^* A)$ by $(A^* A)\,\psi = A^*\,(A\psi)$. Then $A^* A$ is self-adjoint.

A.2 Required Calculus

Lemma A.2.1. *For $\boldsymbol{A} \in \mathbb{R}^{N\times N}$ a symmetric positive definite matrix*

$$\int\limits_{\mathbb{R}^N} g\,(\boldsymbol{z})\, e^{-\frac{1}{2}\boldsymbol{z}^T \boldsymbol{A}^{-1}\boldsymbol{z}}\, d\boldsymbol{z} = \sqrt{\det\,(2\pi \boldsymbol{A})}\, e^{\frac{1}{2}\nabla^T \boldsymbol{A}\nabla} g(\boldsymbol{x})\Big|_{\boldsymbol{x}=\boldsymbol{0}}\ . \tag{A.2.1}$$

Proof. (Sketch) Consider the generalized heat equation

$$u_t - \left(1/2\nabla^T \boldsymbol{A}\nabla\right) u = 0\,, \tag{A.2.2}$$

$$u(0,\boldsymbol{x}) = g(\boldsymbol{x})\,. \tag{A.2.3}$$

Make the change of variables $\widetilde{\boldsymbol{x}} = \sqrt{2}\boldsymbol{A}^{-1/2}\boldsymbol{x}$ which implies

$$\nabla_{\boldsymbol{x}} = \sqrt{2}\boldsymbol{A}^{-1/2}\nabla_{\widetilde{\boldsymbol{x}}}\,.$$

The new equation for $\widetilde{u}\,(t,\widetilde{\boldsymbol{x}}) = u\left(t, \boldsymbol{A}^{1/2}\widetilde{\boldsymbol{x}}\right)$ is

$$\widetilde{u}_t + \left(\frac{1}{2}\nabla^T_{\widetilde{\boldsymbol{x}}}\sqrt{2}\boldsymbol{A}^{-1/2}\boldsymbol{A}\boldsymbol{A}^{-1/2}\sqrt{2}\nabla_{\widetilde{\boldsymbol{x}}}\right)\widetilde{u} = \widetilde{u}_t + \nabla^2_{\widetilde{\boldsymbol{x}}}\widetilde{u} = 0 \tag{A.2.4}$$

$$\widetilde{u}\,(0,\widetilde{\boldsymbol{x}}) = g\left(\frac{\boldsymbol{A}^{1/2}\widetilde{\boldsymbol{x}}}{\sqrt{2}}\right)\ . \tag{A.2.5}$$

This equation has a solution given by the standard method of Green's functions

$$\widetilde{u}\left(t,\widetilde{\boldsymbol{x}}\right)=\frac{1}{\left(4\pi t\right)^{N/2}}\int\limits_{\mathbb{R}^N} g\left(\frac{\boldsymbol{A}^{1/2}\boldsymbol{y}}{\sqrt{2}}\right)\exp\left(\frac{-\left|\widetilde{\boldsymbol{x}}-\boldsymbol{y}\right|^2}{4t}\right)d\boldsymbol{y} \tag{A.2.6}$$

$$=\frac{1}{\sqrt{\det\left(2\pi t\boldsymbol{A}\right)}}\int\limits_{\mathbb{R}^N} g\left(\boldsymbol{z}\right)\exp\left(\frac{-\left|\widetilde{\boldsymbol{x}}-\sqrt{2}\boldsymbol{A}^{-1/2}\boldsymbol{z}\right|^2}{4t}\right)d\boldsymbol{z}\,. \tag{A.2.7}$$

Changing back we see

$$u\left(t,\boldsymbol{x}\right)=\frac{1}{\sqrt{\det\left(2\pi t\boldsymbol{A}\right)}}\int\limits_{\mathbb{R}^N} g\left(\boldsymbol{z}\right)\exp\left(-\frac{1}{2t}\left(\boldsymbol{x}-\boldsymbol{z}\right)^T\boldsymbol{A}^{-1}\left(\boldsymbol{x}-\boldsymbol{z}\right)\right)d\boldsymbol{z}.$$

But, in the semi-group form this is also given as

$$u\left(t,\boldsymbol{x}\right)=e^{\frac{1}{2}\nabla^T\boldsymbol{A}\nabla t}g(\boldsymbol{y})\Big|_{\boldsymbol{y}=\boldsymbol{x}}.$$

Evaluating at $t=1$ and $\boldsymbol{x}=\boldsymbol{0}$ gives us the required relation. □

A.3 Properties of S

Definition A.3.1. *Consider the formal definition of an entropy S*

$$S\left(\eta\right)=\theta\log\left[\int\limits_{\mathcal{Q}}\exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N}m_j\eta\left(q_j\right)-\Phi\left(\boldsymbol{q}\right)\right)\right)d\boldsymbol{q}\right]. \tag{A.3.1}$$

Remark A.3.1. We must identify the class of functions η for which this formula makes sense. Note that at the least we must require $\eta\in L_\infty\left[\mathbb{T}\right]$ since it is possible to provide an example $\eta\in L_p\left[\mathbb{T}\right]$ for any finite p for which $\exp\left(\eta\right)$ is not integrable. For example consider $\eta(x)=\log\left(1/x\right)$.

Lemma A.3.1. *$S:L_\infty\left[\mathbb{T}\right]\to\mathbb{R}$ is convex.*

Proof. We examine $S\left(\lambda\eta_1 + (1-\lambda)\,\eta_2\right)$ for $\lambda \in (0,1)$. First,

$$\exp\left(\frac{1}{\theta}S\left(\lambda\eta_1 + (1-\lambda)\,\eta_2\right)\right) = \int\limits_{\mathcal{Q}} \left(\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\eta_1\left(q_j\right)\right)\right)^{\lambda} \times \left(\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\eta_2\left(q_j\right)\right)\right)^{1-\lambda} \exp\left(-\frac{1}{\theta}\Phi\left(\boldsymbol{q}\right)\right)\, d\boldsymbol{q}\,. \quad \text{(A.3.2)}$$

For the moment consider the integral on the right-hand side of this equation. As discussed above $\mathcal{Q}$ is a compact smooth manifold. We place the measure μ on this space defined by

$$\mu\left(A\right) = \int\limits_{A} \exp\left(-\frac{1}{\theta}\Phi\left(\boldsymbol{q}\right)\right)\, d\boldsymbol{q}\,. \quad \text{(A.3.3)}$$

With this measure we may add to $\mathcal{Q}$ the standard Borel sets on a smooth manifold $\mathcal{B}$ to obtain the compact measure space $(\mathcal{Q}, \mathcal{B}, \mu)$. Now for $\eta_i \in L_\infty\left[\mathbb{T}\right]$ the functions $f, g : \mathcal{Q} \to \mathbb{R}$ defined by

$$f(\boldsymbol{q}) = \left(\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\eta_1(q_j)\right)\right)^{\lambda}, \quad \text{(A.3.4)}$$

$$g(\boldsymbol{q}) = \left(\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\eta_2(q_j)\right)\right)^{1-\lambda}, \quad \text{(A.3.5)}$$

are bounded and measurable and so we may apply the well-known Hölder inequality

$$\left|\left|fg\right|\right|_1 \leq \left|\left|f\right|\right|_p \left|\left|g\right|\right|_q\,, \quad \text{(A.3.6)}$$

where

$$\left|\left|h\right|\right|_p = \left(\int\limits_{\mathcal{Q}} \left(h(\boldsymbol{q})\right)^p \exp\left(-\frac{1}{\theta}\Phi(\boldsymbol{q})\right)\, dq\right)^{1/p}, \quad \text{(A.3.7)}$$

for $1 \leq p < \infty$. We choose $p = 1/\lambda$ so that $\lambda = 1/p$ and $1 - \lambda = 1/q$ to see

$$\int_{\mathcal{Q}} \left(\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j \eta_1\left(q_j\right)\right)\right)^{\lambda} \left(\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j \eta_2\left(q_j\right)\right)\right)^{1-\lambda} d\mu$$
$$\leq \left(\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j \eta_1(q_j)\right) d\mu\right)^{\lambda} \left(\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j \eta_2(q_j)\right) d\mu\right)^{1-\lambda} . \tag{A.3.8}$$

Hence, (since $\log(\cdot)$ is increasing)

$$S(\lambda\eta_1 + (1-\lambda)\,\eta_2) \leq \lambda S(\eta_1) + (1-\lambda)\,S(\eta_2)\,. \tag{A.3.9}$$

$\square$

Lemma A.3.2. $S : L_\infty\left[\mathbb{T}\right] \to \mathbb{R}$ *is Fréchet Differentiable.*

Proof. Consider the linear operator $A_\eta : L_\infty\left[\mathbb{T}\right] \to \mathbb{R}$

$$A_\eta h = \int_{\mathcal{Q}} \sum_{j=1}^{N} m_j h(q_j) \underbrace{\frac{\exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(q_j) - \Phi(\boldsymbol{q})\right)\right)}{\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\left(\sum_{j=1}^{N} m_j \eta(\widetilde{q}_j) - \Phi(\widetilde{\boldsymbol{q}})\right)\right) d\widetilde{\boldsymbol{q}}}}_{:=\mathcal{G}(\boldsymbol{q})} d\boldsymbol{q}\,. \tag{A.3.10}$$

A_η is continuous since

$$|A_\eta h| \leq \sum_{j=1}^{N} m_j \left|\left|h\right|\right|_\infty . \tag{A.3.11}$$

Now define $R\left(\eta, h\right) = S\left(\eta + h\right) - S\left(\eta\right) - A_\eta h$. I will show that

$$\frac{|R(\eta,h)|}{||h||_\infty} \to 0 \text{ uniformly in } \eta \text{ as } \left|\left|h\right|\right|_\infty \to 0\,. \tag{A.3.12}$$

We begin by writing

$$R(\eta,h) = \theta \log\left[\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\right) \mathcal{G}(\boldsymbol{q})\, d\boldsymbol{q}\right] - \int_{\mathcal{Q}} \sum_{j=1}^{N} m_j h(q_j) \mathcal{G}(\boldsymbol{q})\, d\boldsymbol{q}\,. \tag{A.3.13}$$

Now, by Taylor's Theorem we have

$$\int_{\mathcal{Q}} \exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\right)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q}$$
$$= 1 + \int_{\mathcal{Q}} \frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q} + \int_{\mathcal{Q}} R_1\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\right)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q}\,, \quad \text{(A.3.14)}$$

where $R_1(x) = \frac{1}{2}e^{\xi}x^2$ for some $\xi = \xi(x) \in (0, x)$. This means

$$R_1\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\right) \leq \frac{1}{2}\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\,||h||_\infty\right)\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\right)^2 ||h||_\infty^2\,. \quad \text{(A.3.15)}$$

Also by Taylor's Theorem we have

$$\log\left[1 + \int_{\mathcal{Q}} \frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q} + \int_{\mathcal{Q}} R_1\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\right)\mathcal{G}(\boldsymbol{q})d\boldsymbol{q}\right]$$
$$= \int_{\mathcal{Q}} \frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q} + \int_{\mathcal{Q}} R_1\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\right)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q}$$
$$+ R_2\left(\int_{\mathcal{Q}} \frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q} + \int_{\mathcal{Q}} R_1\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\right)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q}\right)\,, \quad \text{(A.3.16)}$$

where $R_2(x) = -\frac{1}{(1+\xi)^2}\frac{x^2}{2}$ for some $\xi = \xi(x) \in (0, x)$. But, since

$$\left|\int_{\mathcal{Q}} \frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q} + \int_{\mathcal{Q}} R_1\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j h(q_j)\right)\mathcal{G}(\boldsymbol{q})\,d\boldsymbol{q}\right|$$
$$\leq \frac{1}{\theta}\sum_{j=1}^{N} m_j\,||h||_\infty + \frac{1}{2}\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\,||h||_\infty\right)\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\right)^2 ||h||_\infty^2\,, \quad \text{(A.3.17)}$$

we have the last term bounded by

$$\frac{1}{2}\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\,||h||_\infty + \frac{1}{2}\exp\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\,||h||_\infty\right)\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\right)^2 ||h||_\infty^2\right)^2$$
$$\leq \frac{1}{2}\left(\frac{1}{\theta}\sum_{j=1}^{N} m_j\right)^2 ||h||_\infty^2 \exp\left(\frac{2}{\theta}\sum_{j=1}^{N} m_j\,||h||_\infty\right)\left(1 + \frac{1}{\theta}\sum_{j=1}^{N} m_j\,||h||_\infty\right)^2 . \quad \text{(A.3.18)}$$

Finally, we put all this together to find

$$
\begin{aligned}
|R(\eta, h)| \leq & \left| \theta \int\limits_{\mathcal{Q}} R_1 \left(\frac{1}{\theta} \sum_{j=1}^{N} m_j h(q_j) \right) \mathcal{G}(\boldsymbol{q})\, d\boldsymbol{q} \right| \\
& + \frac{1}{2} \left(\frac{1}{\theta} \sum_{j=1}^{N} m_j \right)^2 ||h||_\infty^2 \exp\left(\frac{2}{\theta} \sum_{j=1}^{N} m_j\, ||h||_\infty \right) \left(1 + \frac{1}{\theta} \sum_{j=1}^{N} m_j\, ||h||_\infty \right)^2 \\
\leq & \frac{1}{2\theta} \left(\sum_{j=1}^{N} m_j \right)^2 \exp\left(\frac{1}{\theta} \sum_{j=1}^{N} m_j\, ||h||_\infty \right) ||h||_\infty^2 \\
& + \frac{1}{2} \left(\frac{1}{\theta} \sum_{j=1}^{N} m_j \right)^2 ||h||_\infty^2 \exp\left(\frac{2}{\theta} \sum_{j=1}^{N} m_j\, ||h||_\infty \right) \left(1 + \frac{1}{\theta} \sum_{j=1}^{N} m_j\, ||h||_\infty \right)^2 .
\end{aligned}
\tag{A.3.19}
$$

This completes the proof. □

A.4 Properties of $\boldsymbol{\Xi}$

Many of the dynamical aspects of our model rely on the properties of the matrix $\boldsymbol{\Xi}$. For now the only constraint we place upon $\boldsymbol{\Xi}$ is that the elements of $\boldsymbol{\Lambda}$ be strictly positive. First note that since $\boldsymbol{\Xi} = (\boldsymbol{\Lambda\Omega})^T (\boldsymbol{\Lambda\Omega})$ we must have

$$
\mathrm{Null}\,(\boldsymbol{\Xi}) = \mathrm{Null}\,(\boldsymbol{\Lambda\Omega}) = \mathrm{Null}\,(\boldsymbol{\Omega}) = \mathrm{span}\,\{\mathbf{1}\}\ , \tag{A.4.1}
$$

where $\mathbf{1} = (1, 1, \ldots, 1)$. Note also that the form of $\boldsymbol{\Xi}$ makes it clear that the matrix is positive semi-definite.

Also, we can note that the units of $\boldsymbol{\Xi}$ are $\frac{\text{mass}}{\text{time}}$ since from equation (2.1.5)

$$
\mathrm{Units}\,(\boldsymbol{\Xi} \nabla_{\boldsymbol{p}} H) = \mathrm{Units}\left(\frac{\boldsymbol{p}}{t} \right), \tag{A.4.2}
$$

$$
\mathrm{Units}\,(\boldsymbol{\Xi})\, \frac{\text{mass}\frac{\text{length}^2}{\text{time}^2}}{\text{mass}\frac{\text{length}}{\text{time}}} = \frac{\text{mass}\frac{\text{length}}{\text{time}}}{\text{time}}, \tag{A.4.3}
$$

$$
\mathrm{Units}\,(\boldsymbol{\Xi}) = \frac{\text{mass}}{\text{time}} . \tag{A.4.4}
$$

The units and the way $\boldsymbol{\Xi}$ appears in equation (2.1.5) suggests the appropriate inner product space for analyzing $\boldsymbol{\Xi}$ has weight $\boldsymbol{M}^{-1}$ which would make the appropriate eigenstructure the one given by

$$\boldsymbol{\Xi} e_\nu = \nu \boldsymbol{M} e_\nu \,, \tag{A.4.5}$$

where $e_{\nu,i}$ is periodic in i.

Lemma A.4.1. *For the simplest case $\boldsymbol{M} = m_0 \boldsymbol{I}$, $\boldsymbol{\Lambda} = \lambda_0 \boldsymbol{I}$ the eigenvalues solving (A.4.5) satisfy*

$$\nu_k = \frac{2\lambda_0^2}{m_0}\left(1 - \left|\cos\left(\frac{2\pi k}{N}\right)\right|\right) \,, \tag{A.4.6}$$

for $k = 0, 1, \ldots, N-1$.

Proof. Equation (A.4.5) becomes

$$\begin{aligned}
\lambda_0^2\left[2e_{\nu,1} - e_{\nu,2} - e_{\nu,N}\right] &= \nu m_0 e_{\nu,1} \,, \\
\lambda_0^2\left[2e_{\nu,2} - e_{\nu,3} - e_{\nu,1}\right] &= \nu m_0 e_{\nu,2} \,, \\
&\vdots \\
\lambda_0^2\left[2e_{\nu,l} - e_{\nu,l+1} - e_{\nu,l-1}\right] &= \nu m_0 e_{\nu,l} \,, \qquad \text{(A.4.7)} \\
&\vdots \\
\lambda_0^2\left[2e_{\nu,N} - e_{\nu,1} - e_{\nu,N-1}\right] &= \nu m_0 e_{\nu,N} \,,
\end{aligned}$$

a 2$^{\text{nd}}$ order recurrence relation with periodic boundary conditions. Define

$$\beta = 1 - \frac{\nu m_0}{2\lambda_0^2} \,, \tag{A.4.8}$$

and rewrite equation (A.4.7) as

$$2\beta e_{\nu,l} - e_{\nu,l+1} - e_{\nu,l-1} = 0 \,, \tag{A.4.9}$$

which has characteristic equation

$$\xi^2 - 2\beta\xi + 1 = 0\,. \tag{A.4.10}$$

Equation (A.4.10) has roots $\beta \pm \sqrt{\beta^2 - 1}$.

- $\beta = 1$ corresponds to solutions of the form $C_1 + lC_2$ which could only be the trivial constant solution,
- $\beta > 1$ cannot satisfy the periodic boundary conditions,

so we are left with $\beta < 1$ which implies

$$\xi = \beta \pm i\sqrt{1-\beta^2} = \exp\left(\pm i \tan^{-1}\left(\frac{\sqrt{1-\beta^2}}{\beta}\right)\right) := \exp\left(\pm i\alpha\right)\,. \tag{A.4.11}$$

Hence, our candidate solution is

$$e_{\nu,l} = C_1 \cos\left(l\alpha\right) + C_2 \sin\left(l\alpha\right)\,. \tag{A.4.12}$$

The periodicity constraint $e_{\nu,1} = e_{\nu,N+1}$ implies

$$\begin{aligned} C_1 \cos\left(\alpha\right) + C_2 \sin\left(\alpha\right) = C_1 &\left[\cos\left(N\alpha\right)\cos\left(\alpha\right) - \sin\left(N\alpha\right)\sin\left(\alpha\right)\right] \\ &+ C_2\left[\cos\left(N\alpha\right)\sin\left(\alpha\right) + \sin\left(N\alpha\right)\cos\left(\alpha\right)\right]\,. \end{aligned} \tag{A.4.13}$$

Comparing coefficients of $C_1 \cos\left(\alpha\right)$, $C_2 \sin\left(\alpha\right)$ on each side we see that we need

$$\sin\left(N\alpha\right) = 0 \quad \text{and} \quad \cos\left(N\alpha\right) = 1\,. \tag{A.4.14}$$

The largest set of αs satisfying these is

$$N\alpha = 2\pi k \text{ for } k = 0, 1, \ldots, N-1. \tag{A.4.15}$$

So, we have

$$\alpha_k = \frac{2\pi k}{N}\,, \tag{A.4.16}$$

$$\frac{\sqrt{1-\beta_k^2}}{\beta_k} = \tan\left(\frac{2\pi k}{N}\right)\,, \tag{A.4.17}$$

$$\beta_k^2 = \frac{1}{1+\tan^2\left(\frac{2\pi k}{N}\right)} = \cos^2\left(\frac{2\pi k}{N}\right)\,, \tag{A.4.18}$$

$$\nu_k = \frac{2\lambda_0^2}{m_0}\left(1-\left|\cos\left(\frac{2\pi k}{N}\right)\right|\right)\,. \tag{A.4.19}$$

□

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